PB84-164128

Pollution Episodic Model
User's Guide

(U.S.) National Oceanic and
Atmospheric Administration, Oak Ridge, TN

Prepared for

Environmental Sciences Research Lab.
Research Triangle Park, NC

Mar 84

U.S. Department of Commerce
National Technical Information Service
NTIS

PB84-164128

EPA-600/8-84-008
March 1984

POLLUTION EPISODIC MODEL
USER'S GUIDE

by

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IAG-AD-13-F-1-707-0

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ENVIRONMENTAL SCIENCES RESEARCH LABORATORY
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RESEARCH TRIANGLE PARK, NORTH CAROLINA 27711

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NATIONAL TECHNICAL
INFORMATION SERVICE
U.S. DEPARTMENT OF COMMERCE
SPRINGFIELD, VA. 22161

TECHNICAL REPORT DATA

(Please read Instructions on the reverse before completing)

1. REPORT NO.
EPA-600/8-84-008

2.

3. RECIPIENT'S ACCESSION NO.
PB8 4 164128

4. TITLE AND SUBTITLE
POLLUTION EPISODIC MODEL USERS'S GUIDE

5. REPORT DATE
March 1984

6. PERFORMING ORGANIZATION CODE

7. AUTHOR(S)
K. Shankar Rao and Martha M. Stevens

8. PERFORMING ORGANIZATION REPORT NO.

9. PERFORMING ORGANIZATION NAME AND ADDRESS
Atmospheric Turbulence and Diffusion Division
National Oceanic and Atmospheric Administration
Oak Ridge, Tennessee 37830

10. PROGRAM ELEMENT NO.
CDTA1D/02-1606 FY-84

11. CONTRACT/GRANT NO.
IAG-AD-13-1-070-0

12. SPONSORING AGENCY NAME AND ADDRESS
Environmental Sciences Research Laboratory - RTP, nc
Office of Research and Development
U.S. Environmental Protection Agency
Research Triangle Park, North Carolina 27711

13. TYPE OF REPORT AND PERIOD COVERED
Final 9/81-4/83

14. SPONSORING AGENCY CODE
EPA/600/09

15. SUPPLEMENTARY NOTES

16. ABSTRACT

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The concentration algorithms used in PEM are specially developed to account for the effects of dry deposition, sedimentation, and first-order chemical transformation. The Gaussian plume-type algorithms for point sources are derived from analytical solutions of a gradient-transfer model. In the limit, when deposition and settling velocities of the pollutants and the chemical transformation rate are zero, these expressions reduce to the familiar Gaussian plume diffusion algorithms. The concentration algorithms for area sources in PEM are derived from an innovative approach based on mass balance considerations. These algorithms are simple, efficient, and accurate. The computer program of the Texas Episodic Model is used as a framework for the development of the PEM program.

17. KEY WORDS AND DOCUMENT ANALYSIS

a. DESCRIPTORS	b. IDENTIFIERS/OPEN ENDED TERMS	c. COSATI Field/Group

18. DISTRIBUTION STATEMENT
RELEASE TO PUBLIC

19. SECURITY CLASS *(This Report)*
UNCLASSIFIED

20. SECURITY CLASS *(This page)*
UNCLASSIFIED

21. NO. OF PAGES
197

22. PRICE

EPA Form 2220-1 (9-73)

NOTICE

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ABSTRACT

The Pollution Episodic Model (PEM) is an urban-scale model designed to predict short-term average ground-level concentrations and deposition fluxes of one or two gaseous or particulate pollutants at multiple receptors. The two pollutants may be non-reactive, or chemically-coupled through a first-order chemical transformation. Up to 300 isolated point sources and 50 distributed area sources may be considered in the calculations. Concentration and deposition flux estimates are made using the mean meteorological data for an hour. Up to a maximum of 24 hourly scenarios of meteorology may be included in an averaging period.

The concentration algorithms used in PEM are specially developed to account for the effects of dry deposition, sedimentation, and first-order chemical transformation. The Gaussian plume-type algorithms for point sources are derived from analytical solutions of a gradient-transfer model. In the limit, when deposition and settling velocities of the pollutants and the chemical transformation rate are zero, these expressions reduce to the familiar Gaussian plume diffusion algorithms. The concentration algorithms for area sources in PEM are derived from an innovative approach based on mass balance considerations. These algorithms are simple, efficient, and accurate. The computer program of the Texas Episodic Model is used as a framework for the development of the PEM program.

When the chemical transformation option is considered, PEM calculates the average surface concentrations and deposition fluxes of both the primary (reactant) and the secondary (reaction product) pollutants. The model also permits a possible direct emission of the secondary pollutant. The deposition and settling velocities of the two species may be different. Either of the species may be a gaseous or particulate pollutant.

PEM is intended for studies of the atmospheric transport, transformation, and deposition of acidic, toxic, and other pollutants in urban areas, and to assess the impact of new sources or source modifications on air quality for regulatory purposes and urban planning. The information in this report is directed to the model user and the programmer.

This User's Guide to PEM was prepared by NOAA's Atmospheric Turbulence and Diffusion Division in partial fulfillment of Interagency Agreement No. AD-13-F-1-707-0 with the U.S. Environmental Protection Agency. Details of the development and testing of the concentration algorithms used in PEM for point and area sources are given in another report prepared under this Interagency Agreement. This work, covering the period September 1981 to March 1983, was completed as of April 30, 1983.

CONTENTS

Abstract iii

Figures vii

Tables viii

Acknowledgements ix

1. MODEL OVERVIEW

1.1 Introduction 1

1.2 Capabilities and Applications 2

1.3 Assumptions and Limitations 3

1.4 Summary of Input Data 5

1.5 Summary of Model Output 7

2. TECHNICAL DISCUSSION

2.1 Theoretical Basis 9

2.2 Point Sources 10

2.2.1 Concentration Algorithms 10

2.2.2 Plume Rise 12

2.2.3 Dispersion Parameters 14

2.2.4 Restrictions on Receptors for Calculations 16

2.3 Area Sources 17

2.3.1 Emission Grid 17

2.3.2 Concentration Algorithms 23

2.3.3 Dispersion Parameters 26

2.4 Receptors 27

2.4.1 Receptor Grid 27

2.4.2 Automatic Grid Selection 28

2.5 Meteorology 34
2.5.1 Atmospheric Stability 34
2.5.2 Wind Speed 35
2.5.3 Wind Direction 37
2.5.4 Mixing Depth 38
3. COMPUTER PROGRAM OVERVIEW
3.1 Basis for PEM Program 40
3.2 Structure of the Program 41
3.3 General Flow of the Program 43
4. PROGRAM USER'S GUIDE
4.1 Summary of Program Input 45
4.2 Details of Program Input 46
4.2.1 Control Parameters 46
4.2.2 Scenario Parameters 52
4.2.3 Area Source Parameters 53
4.2.4 Point Source Parameters 54
4.2.5 Discussion of Input Parameters 55
4.3 Guide to Program Output 58
4.4 Example Problems 60
References 61
Appendices
A. Point Source Algorithms 62
B. Plume Rise Equations 71
C. Surface Deposition Fluxes, and Deposition and Settling Velocities 74
D. D01AJF - NAG FORTRAN Library Routine Document 77
E. Input and Output Listings of Example Problems 81
F. PEM FORTRAN Listing 128

FIGURES

Number		Page
1	Schematic diagram showing a single grid square with emissions and four downwind calculation grid squares with receptors, and the distances used in area-source algorithms	18
2	Spatial patterns of affected calculation grid squares downwind of an area source	20-21
3	Schematic diagram showing a single grid square with receptor and four upwind grid squares with emissions, and the distances used in area-source algorithms	25
4	Points used for automatic selection of receptor grid by AUTGRD subroutine	30
5	Example of a receptor grid selected by AUTGRD subroutine	33
6	Structure of PEM computer program	42

TABLES

Number Page

1 Values of a and b in $\sigma_z = a\ x^b$ for point sources 15

2 Values of c and d in $\sigma_y = c\ x^d$ for point sources 15

3 Maximum crosswind angle values for point source plumes 16

4 Values of i and j for each spatial pattern of affected squares downwind of an area source 19

5 Values of a and b in $\sigma_z = a\ x^b$ for area sources 27

6 Atmospheric stability classes 34

7 Atmospheric conditions defining stability classes 35

8 Wind speed classification 36

9 Values of exponent p in wind speed power law 36

10 Wind direction sectors 37

11 Input data for Example Problem 1 82

12 Output listing for Example Problem 1 83

13 Input data for Example Problem 2 96

14 Output listing for Example Problem 2 97

15 Input data for Example Problem 3 109

16 Output listing for Example Problem 3 110

ACKNOWLEDGEMENTS

This report was prepared for the Office of Research and Development, Environmental Sciences Research Laboratory of the U. S. Environmental Protection Agency to support the needs of EPA's Office of Air Quality Planning and Standards in urban particulate modeling. This work was accomplished under interagency agreements among the U. S. Department of Energy, the National Oceanic and Atmospheric Administration, and the EPA. The authors are grateful to Dr. Jack Shreffler of ESRL for the opportunity to do this work, and for his interest and patience. The authors also express their appreciation to the following members of the Atmospheric Turbulence and Diffusion Division: Director Bruce B. Hicks for his understanding and support, Dr. Ray Hosker for useful suggestions and discussions during the course of this work, and Mrs. Mary Rogers for her expert technical typing and patient revisions. Special thanks are due to Bernadette Kirk, Nancy Price, and Louise Taylor, who worked as programmers for this project at various times and assisted in the development and testing of the concentration algorithms for PEM.

Several figures and tables shown in this report are reproduced from the Users' Guide to Texas Episodic Model with permission from the Texas Air Control Board. The library routine D01AJF used for numerical integration in PEM has been released by the Computer Sciences Division of the Oak Ridge National Laboratory for inclusion in the program listing. The Numerical Algorithms Group holds the copyright to this routine and its document. The latter is reproduced in this report from the NAG FORTRAN Mini-Manual.

SECTION 1

MODEL OVERVIEW

1.1 INTRODUCTION

The Pollution Episodic Model (PEM) is an urban-scale model designed to predict short-term ground-level concentrations and deposition fluxes of one or two gaseous or particulate reactive atmospheric pollutants in an urban area with multiple point and area sources. PEM uses point and area-source concentration algorithms developed by Rao (1982) which explicitly account for the effects of dry deposition, gravitational settling, and a first-order chemical transformation. These algorithms, derived analytically from a gradient-transfer model, are based on Gaussian plume modeling assumptions. The surface concentrations and deposition fluxes of both the primary (reactant) and the secondary (reaction product) pollutants are calculated.

The PEM is based on the Texas Episodic Model (TEM) developed by the Texas Air Control Board (1979) for the atmospheric dispersion of non-reactive pollutants over a perfectly reflecting surface. In the limit, when the deposition and settling velocities and the chemical transformation rate are zero, the point-source concentration algorithms used in PEM reduce to the familiar Gaussian plume dispersion algorithms used in TEM. As this limit is approached, the new area source algorithms used in PEM give essentially the same values as TEM for ground-level concentrations of pollutants. The two models share the same framework for calculations. Some of the key assumptions of TEM, also retained in PEM, are as follows:

1. All area source emissions are assumed to occur at the ground-level. The variation of the vertical dispersion coefficient $\sigma_z(x)$ was expressed by a power law given by Gifford and Hanna (1970). The enhanced near-surface diffusion over urban areas was simulated by decreasing the stability class index by one for all classes except Class A. The horizontal diffusion was ignored for the narrow plumes resulting from distributed area sources.
2. Values for the horizontal and vertical dispersion coefficients, $\sigma_y(x)$ and $\sigma_z(x)$, for point sources were derived from power laws fitted to the empirically-derived Pasquill-Gifford curves given by Turner (1970). Their values were identical to those used in EPA's Climatological Dispersion Model (Busse and Zimmerman, 1973).
3. The wind speed at the anemometer height was adjusted to the stack height using a power law with the exponents given by DeMarrais (1959). The penetration of an inversion layer aloft by a buoyant plume was considered by defining an inversion penetration factor capable of simulating inversions of various strengths.

Some of the important differences between PEM and TEM are listed in Section 3 of this report.

1.2 CAPABILITIES AND APPLICATIONS

The capabilities of PEM are as follows:

1. PEM is an urban-scale model applicable to downwind distances of up to 60 km.
2. Up to a maximum of 300 point sources and 50 area sources can be included in the model inputs to estimate concentrations at a maximum of 2500 receptors located on a 50 x 50 square receptor grid.

3. PEM calculates short-term (1 to 24 hr) average ground-level concentrations and deposition fluxes of one or two gaseous or particulate pollutants.
4. The two pollutants may be non-reactive, or chemically-coupled through a first-order chemical transformation. Either or both of the two pollutants may be gaseous or particulate species.
5. If only one pollutant is calculated, the effects of a first-order chemical decay can be considered.
6. There is no restriction on the size of the particles. The chemical transformation or decay rate may vary from 0.1 to 100 percent per hour.
7. The deposition (and settling) velocities of the two species may be equal or different. Direct emission of the secondary (reaction product) pollutant may be zero or non-zero for point and area sources.

Some areas of potential application of PEM are the following:

1. Urban particulate modeling.
2. Studies of the transport, diffusion, transformation, and deposition of acidic, toxic, and other pollutants in urban areas. An important example is the atmospheric transport and transformation of SO_2 to $SO_4^=$.
3. Impact analyses of new sources or source modifications for regulatory purposes.
4. Stack parameter design studies.
5. Fuel conversion/switching studies. Evaluation of pollution control technology and strategies.
6. Prevention of significant deterioration.
7. Urban planning.

1.3 ASSUMPTIONS AND LIMITATIONS

PEM is based on steady state Gaussian plume modeling assumptions.

Some of the important assumptions of PEM are as follows:

1. The sources are stationary and the emission rates are constant over the concentration-averaging period.

2. Concentration estimates may be made for each hour using the mean meteorological conditions for that hour. Concentrations for a period longer than an hour can be determined by averaging the hourly concentrations of that period. This can be done externally with minimal programming to calculate, for example, 24-hour average concentrations with diurnally varying emission rates.

3. Total concentration at a receptor is the sum of the concentrations calculated at the receptor from each source; i.e., concentrations are additive.

4. Pollutants released from a stack are transported downwind at a rate equal to the mean wind speed at the physical stack height. The wind direction is constant for each hour. The horizontal wind field is homogeneous and the effects of directional wind shear are neglected.

5. Diffusion of continuous plumes gives time-averaged Gaussian distributions for concentrations in the crosswind and vertical directions. The diffusion in the downwind direction is negligible compared to advection.

6. The reactant and the product species are coupled through a first-order chemical transformation. The deposition and settling velocities of the species, and the chemical transformation rate are constant over the concentration-averaging period. The diurnal variation of these parameters can be considered, if necessary, by averaging the hourly concentrations as discussed above.

7. Particulate pollutants consist of particles of a known size (or size distribution) with a representative settling velocity.

8. Pollutant concentration at a receptor due to the distributed area sources depends only on sources located in a narrow upwind sector. Therefore, horizontal diffusion can be ignored for area sources.

9. The crosswind variations of urban area source-strength patterns can be ignored. The contributions of more remote upwind area sources to the concentration at a receptor are quite small. For this reason, it is generally adequate to consider only four area source grid squares immediately upwind of each receptor grid square.

10. The enhanced near-surface diffusion over urban areas is simulated by decreasing the stability class index by one for all classes except Class A. This correction is applied only to distributed urban area sources, assumed to be at ground-level, and not to the isolated point sources, which are generally located at higher elevations.

Every air pollution model is limited by the assumptions used to predict the pollutant concentrations in the atmosphere. PEM is subject to the same basic limitations as any Gaussian plume-type model. The limiting assumptions of the state-of-the-art algorithms developed for PEM are discussed in detail by Rao (1982). Other general limitations of the model can be summarized as follows:

1. Receptors farther than 60 km downwind of a source are ignored. Thus the maximum downwind distance is limited to 60 km.
2. The number of point sources is limited to 300, and the number of area sources is limited to 50. A user can easily expand the maximum number of point and/or area sources, if necessary. All sources are stationary.
3. The maximum number of scenarios (sets of hourly meteorological data) in an averaging period is limited to 24. PEM is designed to calculate only short-term (1 to 24 hr) average surface concentrations and deposition fluxes of one or two pollutants.
4. PEM does not make any adjustment for differences in terrain elevation between sources and/or receptors. The model assumes level terrain.
5. Only a first-order chemical transformation/decay is considered. The transformation rate, and the deposition and settling velocities of the species, should be specified by the user. If area sources are included, the deposition velocities should be nonzero to avoid singularities in the computations.

1.4 SUMMARY OF INPUT DATA

Input to PEM is divided into four main sections:

1) Control parameters

Control parameters remain constant throughout the model run. They specify:

1. An alphanumeric title
2. Time-averaging option
3. Options for types of input and output

4. Number of scenarios (sets of hourly meteorological data)
5. Stack-tip downwash option for point sources
6. Receptor grid coordinates and spacing
7. Automatic receptor grid option
8. Potential temperature gradient $d\theta/dz$ for calculation of plume rise with E and F atmospheric stability classes
9. Parameters for one or two pollutants
    a. Deposition velocity
    b. Gravitational settling velocity
10. Option to calculate chemical transformation or decay for first pollutant
    a. Chemical transformation or decay rate
    b. Ratio of molecular weights of product to reactant
11. Scaling factors for area source emission rates
12. Calibration coefficients to be applied to the calculated concentrations
13. Alphanumeric labels for pollutants
14. Alphanumeric labels for the calibrated concentrations

2) Scenario Parameters

A scenario is a set of mean meteorological data for one hour. From one to twenty-four scenarios may be included in each run. Each scenario uses the same receptor grid and the same point and area source inventories. Meteorological parameters for each scenario are

1. Atmospheric stability class
2. Wind speed class or specific wind speed
3. Wind direction sector or specific wind direction
4. Ambient temperature
5. Inversion penetration factor
6. Mixing height

3) Area Source Inventory

From zero to fifty area sources may be included in each run. Each area source square is described by:

1. Location in receptor grid coordinates
2. Length of a side
3. Emission rates for pollutants

4) Point Source Inventory

From zero to three hundred point sources may be included in each run. Each point source is described by:

1. Location in receptor grid coordinates
2. Emission rates for pollutants
3. Stack height
4. Inside exit diameter of the stack
5. Exit velocity of the plume
6. Exit temperature of the plume
7. Alphanumeric identification

Details of the input data to PEM are given in Section 4 of this report.

1.5 SUMMARY OF MODEL OUTPUT

For ease of reference, PEM output lists and briefly explains all input control parameters used in a run. Input data for meteorological conditions, area sources, and point sources are also listed.

Calculated values of surface concentrations, deposition fluxes, and other useful information may be displayed in the following optional forms:

1. List Option --- For each receptor in the grid, the calculated values of concentrations and deposition fluxes are listed for each scenario.

2. Spatial Array Option --- The calculated values of concentrations and deposition fluxes at each receptor are displayed in map form for each scenario.

3. Tape Option --- The calculated values of concentrations and deposition fluxes at each receptor are written on a magnetic tape (designated for output) for each scenario. This option may be used to generate inputs to a contour-plotting routine.

4. Culpability List Option --- The five point sources which contributed most to the total concentration at each receptor are identified by point-source sequence number. A list of these source numbers and their percent contributions are printed for each receptor in the grid for each scenario. This option may be used only when the model calculates concentrations of a single pollutant.

5. Maximum Concentration Option --- The maximum calculated values of surface concentration and deposition flux for each scenario, and the receptor where these values occur, are printed for each pollutant at the end of the run.

6. Point Source List Option --- The input stack parameters, the wind speed at physical stack height, the maximum effective source height and the dominant plume rise influence are listed for each point source.

These output options are selected by the user by specifying appropriate values for the control parameters in the inputs to the model. It may not be possible to elect some of these options in combination with the others. The details are discussed in Section 4.

SECTION 2

TECHNICAL DISCUSSION

2.1 THEORETICAL BASIS

The concentration algorithms used in PEM are derived from analytical solutions of a steady state gradient-transfer (K-theory) model, which describes the atmospheric transport, diffusion, deposition, and first-order chemical transformation of gaseous or particulate pollutants from an elevated continuous point source. The eddy diffusivity coefficients in these analytical solutions are expressed in terms of the empirical Gaussian plume dispersion parameters, so that the latter can be conveniently specified as functions of the downwind distance and the atmospheric stability class within the framework of the standard turbulence-typing schemes. The point-source concentration algorithms for the primary (reactant) and the secondary (product) pollutants are presented for various stability and mixing conditions of the atmosphere. In the limit when deposition and settling velocities and the chemical transformation rate are zero, these algorithms reduce to the well-known Gaussian plume dispersion algorithms presently used in EPA air quality models. Details of the gradient-transfer model formulations, analytical solutions, parameterizations, and development of the point-source concentration algorithms can be found in the reports by Rao (1982, 1981).

The PEM algorithms for ground-level concentrations of the primary and secondary pollutants resulting from urban area source emissions are derived from an innovative mathematical approach based on mass budgets of the species. These expressions for area sources involve only the point-source algorithms for the well-mixed region; this permits the use of the same subroutines for both point and area sources in the PEM computer program. Thus, the area-source concentration algorithms used in PEM are simple, efficient, and accurate. Details of their mathematical derivation, physical interpretation, and application to multiple urban area sources and receptors can be found in the report by Rao (1982).

PEM uses Briggs' (1969, 1975) plume rise formulations for point sources, empirically-derived Pasquill-Gifford dispersion parameters (Gifford, 1968, 1976), and the urban area-source modeling techniques due to Gifford and Hanna (1970).

2.2 POINT SOURCES

2.2.1 Concentration Algorithms

The ground-level concentrations of the primary and the secondary pollutants (denoted by subscripts 1 and 2, respectively) from an elevated continuous point source are calculated in PEM from one or both of the following sets of algorithms, depending on the atmospheric stability and mixing conditions:

Near-source region $(0 < x \leqq x_m)$,

$$C_1 = \frac{Q_1}{U} \cdot \frac{g_1}{L_y} \cdot \frac{g'_{21}}{L_z} \tag{1a}$$

$$C_2 = \frac{Q_1}{U} \cdot \frac{g_1}{L_y} \cdot \frac{g'_{22}}{L_z} \tag{1b}$$

Well-mixed region $(x \geqq 2\, x_m)$,

$$C_1 = \frac{Q_1}{U} \cdot \frac{g_1}{L_y} \cdot \frac{g'_{41}}{L} \tag{2a}$$

$$C_2 = \frac{Q_1}{U} \cdot \frac{g_1}{L_y} \cdot \frac{g'_{42}}{L} \tag{2b}$$

$$L_y = \sqrt{2\pi}\, \sigma_y \; , \; L_z = \sqrt{2\pi}\, \sigma_z \tag{3}$$

In the above, Q_1 is emission rate (source strength) of the primary pollutant, U is mean wind speed at physical stack height, L is mixing depth (height of inversion lid), x_m is the downwind distance (from source) at which $\sigma_z(x_m) = 0.47\, L$, and L_y and L_z are length scales characteristic of diffusion in the horizontal crosswind and vertical directions, respectively. The nondimensional functions $g_1(\hat{x},\hat{y})$, $g'_{21}(\hat{x},0)$, $g'_{22}(\hat{x},0)$, $g'_{41}(\hat{x})$, and $g'_{42}(\hat{x})$, defined in terms of dimensionless parameterized variables, are given in Appendix A.

In Eqs. (1) and (2), it should be noted that the concentrations for both primary and secondary pollutants are expressed in terms of Q_1. This does not preclude consideration of a non-zero value for Q_2, the direct emission rate of the secondary pollutant. The algorithms g'_{22} and g'_{42} provide for this possibility.

The well-mixed region algorithms, Eq. (2), are generally used under convective or neutral stability conditions. The ground-level plume centerline concentrations of the species in the plume-trapping region ($x_m < x < 2x_m$) can be obtained by calculating the concentrations at x_m and $2x_m$ from Eqs. (1) and (2), and interpolating between these values on a log-log plot of concentrations versus downwind distance (Turner, 1970). PEM uses this interpolation approach in the plume-trapping region.

2.2.2 Plume Rise

Plume rise is calculated from equations given by Briggs (1969, 1975). The stack-exit conditions of the plume and the ambient temperature determine whether the upward motion of the plume is dominated by momentum or buoyancy. For atmospheric stability classes A to D, the unstable/neutral plume rise equations are used. For stability classes E and F, the stable plume rise equations are used. Thus, there are four different situations for plume rise: (1) unstable/neutral atmosphere with buoyancy-dominated plume, (2) stable atmosphere with buoyancy-dominated plume, (3) unstable/neutral atmosphere with momentum-dominated plume, and (4) stable atmosphere with momentum-dominated plume. In each situation except the last one, the plume rise is calculated as a function of downwind distance from the source until the final plume rise is attained. The equations for these four cases are given in Appendix B.

For a given atmospheric stability class for each scenario, PEM calculates both momentum and buoyancy-dominated maximum plume rises for each stack. Based on the higher of these two values, the appropriate plume-rise equation is selected and used to calculate the plume rise, $\Delta h(x)$, for each stack. The effective source height, H, is then obtained from $H = h_s + \Delta h$, where h_s is the physical stack height.

Following Briggs (1973), PEM provides an option to account for stack-tip downwash effects on the effective stack height. When the stack-exit velocity (V) of the plume is less than 1.5 times the mean wind speed (U) at the physical stack height, the stack-tip downwash correction term, H_c, is calculated as

$$H_c = 2\ (1.5 - \frac{V}{U})\ d \qquad (4)$$

where d is the inside diameter of the stack-tip. This value of H_c is subtracted from the effective stack height H. When this option is used, care should be taken to see that H_c has the same units as H.

2.2.3 Dispersion Parameters

The Gaussian dispersion parameters, σ_y and σ_z, used in PEM for each hourly scenario, are identical to those used in EPA's Climatological Dispersion Model (Busse and Zimmerman, 1973) to represent a 1-hour average dispersion, and in the Texas Episodic Model (TACB, 1979) to represent a 10-minute average dispersion from point sources. The values of these parameters are calculated from power laws fitted to the Pasquill-Gifford empirical data curves (Turner, 1970; Gifford, 1976), as follows:

$$\sigma_z(x) = a\ x^b \tag{5a}$$

$$\sigma_y(x) = c\ x^d \tag{5b}$$

The values of a and b used in PEM for point sources are shown in Table 1 as functions of the atmospheric stability class and the downwind distance. The values of c and d are shown in Table 2. Unlike the TEM, the σ_y values in PEM are not adjusted for horizontal meander of the plume since they are assumed to represent 1-hour average dispersion.

It should be noted that the Pasquill-Gifford curves were derived from measurements taken in open, level to gently rolling terrain, and may not be the best estimate of dispersion coefficients for urban areas or rough terrain. The diffusion over cities is enhanced, compared to that over rural areas, due to increased mechanical and thermal turbulence resulting from the larger surface roughness and heat capaicty of the cities. This is reflected in the urban dispersion parameter curves based on interpolation formulas given by Briggs (see Gifford, 1976, Figure 7).

TABLE 1

Values of a and b in $\sigma_z = a\ x^b$ for Point Sources

Atmospheric Stability Class	Downwind Distance (meters)					
	$100 < x \leq 500$		$500 < x \leq 5000$		$5000 < x$	
	a	b	a	b	a	b
A=1	.0383	1.281	.0002539	2.089	.0002539	2.089
B=2	.1393	.9467	.04936	1.114	.04936	1.114
C=3	.1120	.9100	.1014	.926	.1154	.9109
DD=4	.0856	.8650	.2591	.6869	.7368	.5642
DN=5	.0818	.8155	.2527	.6341	1.2970	.4421
E=6	.1094	.7657	.2452	.6358	.9204	.4805
F=7	.05645	.8050	.1930	.6072	1.5050	.3662

TABLE 2

Values of c and d in $\sigma_y = c\ x^d$ for Point Sources

Atmospheric Stability Class	Downwind Distance (meters)			
	$x < 10,000$		$x \geq 10,000$	
	c	d	c	d
A=1	.495	.873	.606	.851
B=2	.310	.897	.523	.840
C=3	.197	.908	.285	.867
DD=4	.122	.916	.193	.865
DN=5	.122	.916	.193	.865
E=6	.0934	.912	.141	.868
F=7	.0625	.911	.080	.884

2.2.4 Restrictions on Receptors for Calculations

Pollutants from each point source may not contribute to all of the receptors in a grid. The receptors excluded from calculations are those located upwind of the source, too far from the plume centerline, or more than 60 km downwind of the source. For each source and each scenario, PEM selects a rectangular area of the receptor grid downwind of the source, and calculations for that set of conditions are restricted to the receptors located within that area. The source contribution is considered to be zero at receptors located outside the area. Model inputs used for determining this area are the source coordinates, grid boundaries, wind direction, and the crosswind angle (Δ) between wind direction azimuth and the azimuth from the source to the receptor. If Δ exceeds the maximum crosswind angle of the plume (Δ_{max}), then the receptor is excluded from calculations. The values of the maximum crosswind angle used in PEM for 1-hour averaging of the plume are shown in Table 3 as a function of the atmospheric stability class.

TABLE 3

Maximum Crosswind Angle Values
for Point Source Plumes

Atmospheric Stability Class	Δ_{max} (degrees)
A	35
B	28
C	21
DD and DN	14
E	10.5
F	7

2.3 AREA SOURCES

2.3.1 Emission Grid

PEM defines a "calculation grid" by shifting the receptor grid to the South and to the West by one-half the side of a grid square ($\Delta x/2$). Thus each square in the calculation grid has one receptor at its center, since the calculation grid squares are of the same size (Δx) as the receptor grid squares.

Each area source used in PEM should be sized so that it covers an integral number of calculation grid squares. The size Δx should be defined such that the smallest area source is at least as large as one calculation grid square.

The relationship between area sources and calculation grid squares can be divided into three cases. In the first case, the area source is the size of a calculation grid square. Emissions (Q_o) are assumed to be located at the center of the square; contributions of this area source are determined at the receptor (R_o) located at the center of the emission grid square, and at the receptors (R_1 to R_4) located at the center of each of the four calculation grid squares immediately downwind of the source. This is schematically illustrated in Fig. 1.

The location of the four downwind squares is not apparent in cases when the wind direction is not parallel to one of the calculation grid

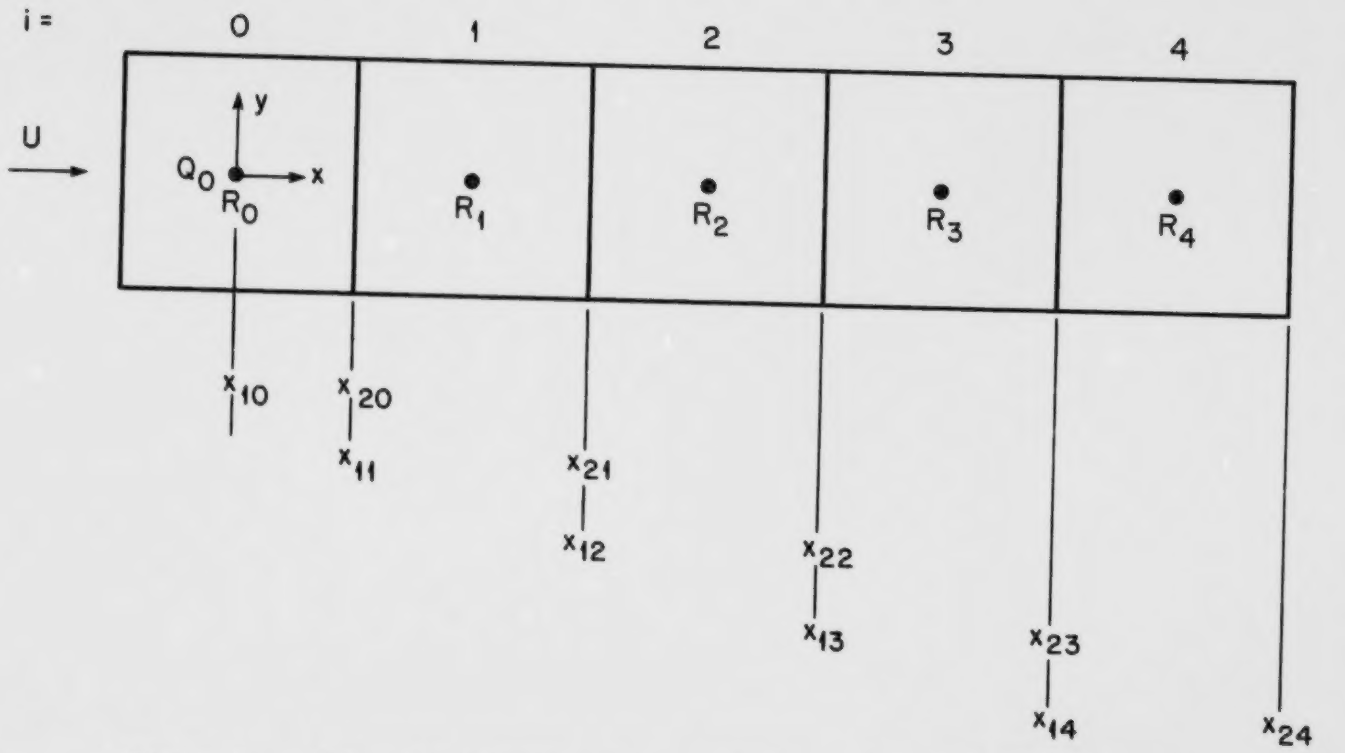

i =
0
1
2
3
4
U
y
x
Q_0
R_0
R_1
R_2
R_3
R_4
x_{10}
x_{20}
x_{11}
x_{21}
x_{12}
x_{22}
x_{13}
x_{23}
x_{14}
x_{24}

Figure 1. Schematic diagram showing a single grid square with emissions and four downwind calculation grid squares with receptors, and the distances used in area-source algorithms. These distances are measured downwind from the source Q_o.

coordinate axes as shown in Fig. 2. The angle between the wind azimuth and the nearest calculation grid coordinate axis is defined as ξ, so $0° \leqq \xi \leqq 45°$. PEM considers ten ranges of values for ξ as shown in Table 4. For each range of ξ, the location of the four downwind squares is shown in Fig. 2. For each

TABLE 4

Values of i and j for Each Spatial Pattern
of Affected Squares Downwind
of an Area Source

ξ range, degrees	Values for j**				
	i=0*	i=1	i=2	i=3	i=4
0 - 7.12	0	0	0	0	0
7.12 - 9.46	0	0	0	0	1
9.46 - 14.04	0	0	0	1	1
14.04 - 20.56	0	0	1	1	1
20.56 - 26.57	0	0	1	1	2
26.57 - 32.01	0	1	1	2	2
32.01 - 36.87	0	1	1	2	3
36.87 - 39.81	0	1	2	2	3
39.81 - 41.19	0	1	2	3	3
41.19 - 45.00	0	1	2	3	4

*i is the number of calculation grid squares downwind from the area source

**j is the number of calculation grid squares from the axis used to define ξ

For each value of ξ, a diagram of the downwind squares is shown in Figure 2.

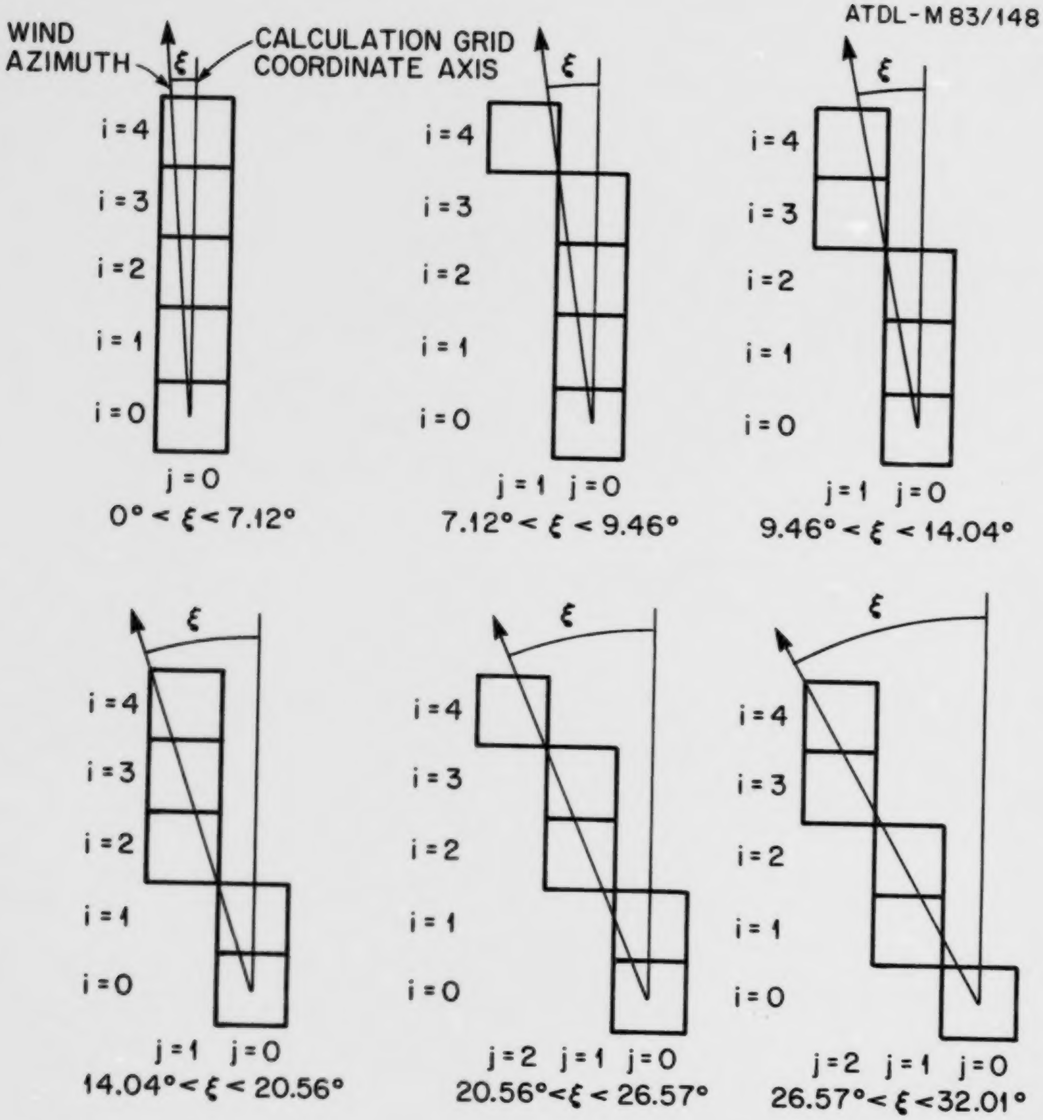
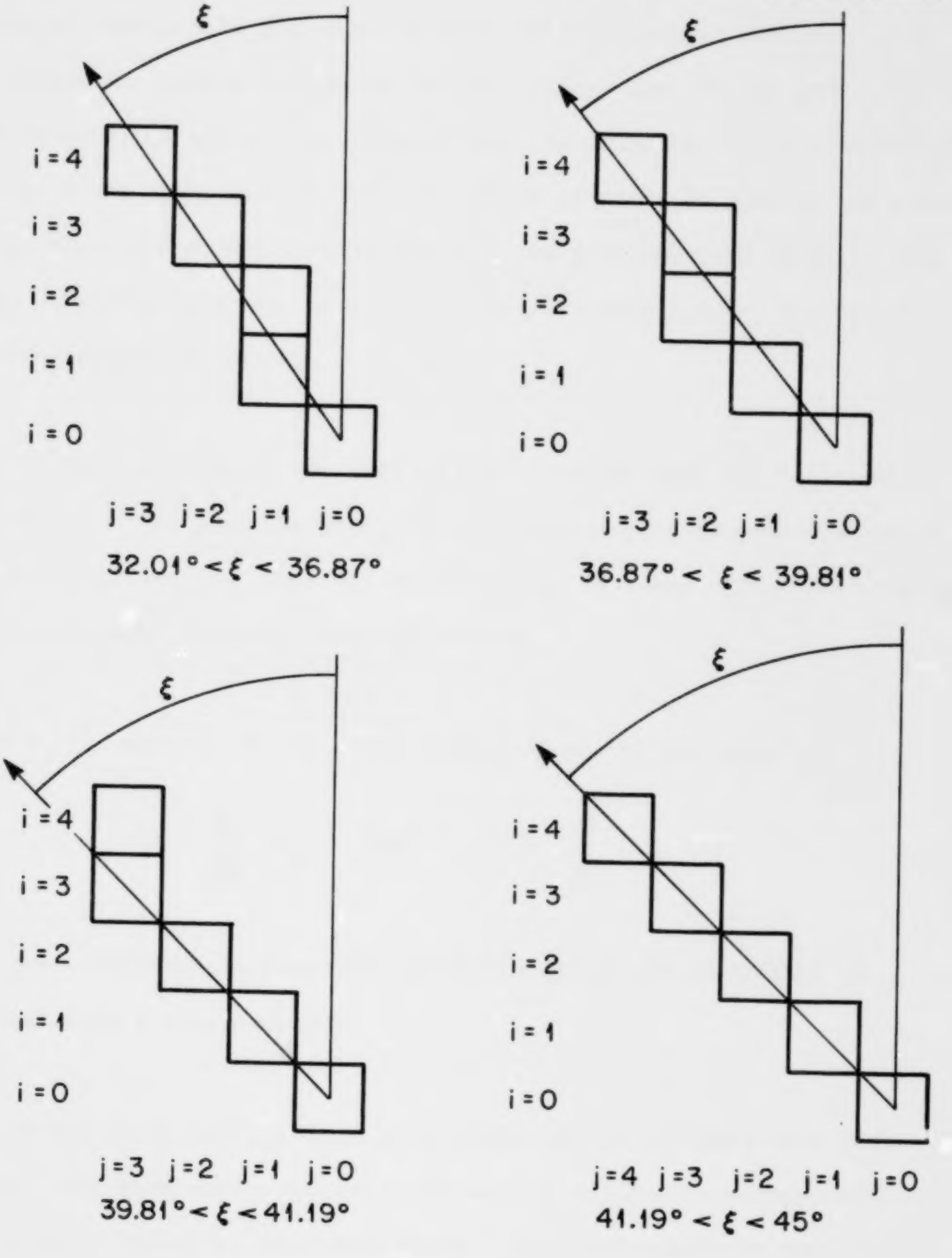

ATDL-M 83/148
WIND AZIMUTH
CALCULATION GRID COORDINATE AXIS
ξ
i=4
i=3
i=2
i=1
i=0
j=0
0° < ξ < 7.12°
j=1 j=0
7.12° < ξ < 9.46°
j=1 j=0
9.46° < ξ < 14.04°
j=1 j=0
14.04° < ξ < 20.56°
j=2 j=1 j=0
20.56° < ξ < 26.57°
j=2 j=1 j=0
26.57° < ξ < 32.01°

Figure 2. Spatial patterns of affected calculation grid squares downwind of an area source.


ξ
i = 4
i = 3
i = 2
i = 1
i = 0
j = 3 j = 2 j = 1 j = 0
ξ
i = 4
i = 3
i = 2
i = 1
i = 0
j = 3 j = 2 j = 1 j = 0
ξ
i = 4
i = 3
i = 2
i = 1
i = 0
j = 3 j = 2 j = 1 j = 0
ξ
i = 4
i = 3
i = 2
i = 1
i = 0
j = 4 j = 3 j = 2 j = 1 j = 0

$32.01° < \xi < 36.87°$

$36.87° < \xi < 39.81°$

$39.81° < \xi < 41.19°$

$41.19° < \xi < 45°$

Figure 2. Continued

value of ξ, the location of each downwind square is denoted by i (the number of calculation grid squares downwind from the area source) and j (the number of calculation grid squares from the axis used to define ξ). In all cases, the square covered by the area source has i=0 and j=0. For each value of i, values for j depend upon the value for ξ, as illustrated in Fig. 2 and summarized in Table 4. These patterns of squares are stored in PEM data tables that list values of i and j as shown in Table 4. For a given scenario, each area source will have the same spatial pattern of affected squares downwind.

In the second case, the area source is larger than one calculation grid square. Let m be the number of calculation grid squares covered by the source of area A. Then the emissions, Q, from the source are divided into m component emission rates defined by

$$Q_j = Q\,A_j/A \quad , \quad j = 1,2,\ \ldots,\ m$$

where A_j is the area of the source contained in the jth square,

$$A = \sum_{j=1}^{m} A_j \qquad \text{and} \qquad Q = \sum_{j=1}^{m} Q_j .$$

Then the contributions from each of the m squares are determined as was done from a single square.

In the third case, a small area source may be imbedded in a large area source. For each source the emission rate is divided into components for each covered square as described above. Then each square is considered as an area source with an emission rate equal to the sum of the component emission rates from the original area sources.

Here, $g'_{41}(\hat{x})$ and $g'_{42}(\hat{x})$ are point-source concentration algorithms for the well-mixed region. These nondimensional functions, and other dimensionless parameters (capped quantities) in this equation, are defined in Appendix A; x_{1i} and x_{2i} are distances measured from Q_o to the upwind and downwind edges, respectively, of the calculation grid square with the ith receptor (see Fig. 1); $\hat{x}_{1i}$ and $\hat{x}_{2i}$ are the corresponding dimensionless values; τ_c is characteristic time scale of the first-order chemical transformation, and $\hat{\tau}_c$ is its dimensionless value as defined in Appendix A; γ is the ratio of molecular weights of the product species to the reactant species; V_{d1} and V_{d2} are deposition velocities of the primary and secondary pollutants, respectively; b is the value of the exponent in the power-law,

$$\sigma_z(x) = a\ x^b \tag{7}$$

for area sources.

Now let us consider five area sources, located upwind of a single receptor R_o in i=0th grid square, as shown in Fig. 3. The total surface concentrations at the receptor in this case can be obtained by summing up the individual contributions of all five area sources, as follows:

$$C_{A1} = \frac{1}{2(1-b)V_{d1}} \sum_{i=0}^{4} Q_{1i} \left[g'_{41}(\hat{x}_{1i}) - g'_{41}(\hat{x}_{2i}) - \frac{1}{\hat{\tau}_c} \int_{\hat{x}_{1i}}^{\hat{x}_{2i}} g'_{41}(\hat{x})d\hat{x} \right] \tag{8a}$$

$$C_{A2} = \frac{1}{2(1-b)V_{d2}} \sum_{i=0}^{4} Q_{1i} \left[g'_{42}(\hat{x}_{1i}) - g'_{42}(\hat{x}_{2i}) + \frac{\gamma}{\hat{\tau}_c} \int_{\hat{x}_{1i}}^{\hat{x}_{2i}} g'_{41}(\hat{x})d\hat{x} \right] \tag{8b}$$

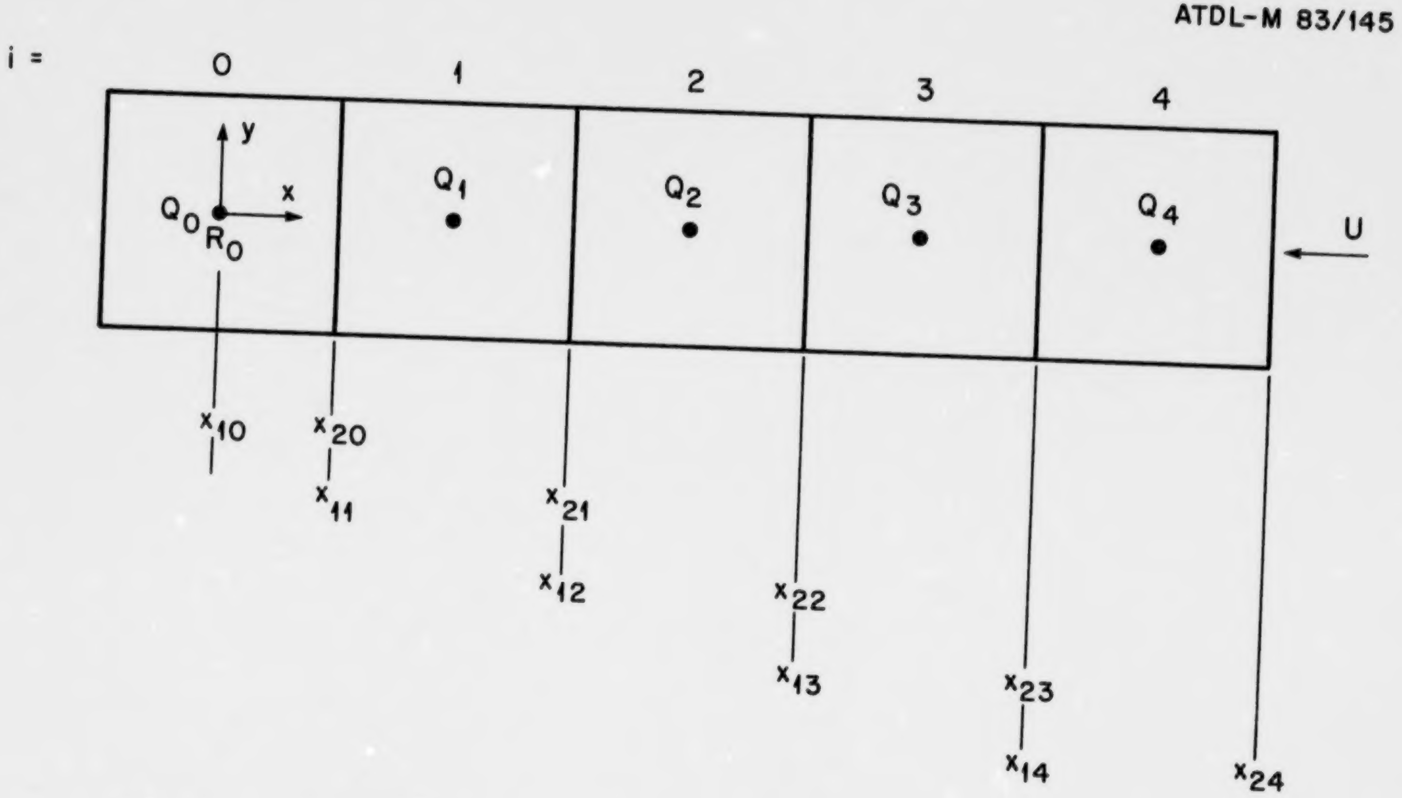

ATDL-M 83/145
i =
0
1
2
3
4
y
x
Q_0
R_0
Q_1
Q_2
Q_3
Q_4
U
x_{10}
x_{20}
x_{11}
x_{21}
x_{12}
x_{22}
x_{13}
x_{23}
x_{14}
x_{24}

Figure 3. Schematic diagram showing a single grid square with receptor and four upwind grid squares with emissions, and the distances used in area-source algorithms. These distances are measured upwind from the receptor R_o.

Here x_{1i} and x_{2i} are the distances measured from the receptor R_o to the downwind and upwind edges, respectively, of the ith emission grid square, as shown in Fig. 3. Note that these distances are identical to those used in Eq. (6), since all grid squares are equal in size. The multiple-source algorithms, Eq. (8), can be easily adapted to calculate concentrations at multiple receptors. For details, the user is referred to Rao (1982).

2.3.3 Dispersion Parameters

It should be noted that the area source concentration algorithms, given above, ignore horizontal diffusion. Gifford (1959) postulated that concentration at a receptor due to the distributed area sources depends only on sources located in a rather narrow upwind sector. The horizontal width of this sector is generally much less than the usual 22.5° resolution of observed wind directions. Consequently, horizontal diffusion can be ignored. This assumption is also referred to as the "narrow plume hypothesis."

The vertical dispersion parameter is given by Eq. (7). The coefficients a and b are functions only of atmospheric stability. Their values, based on extensive observational data, can be found in various texts, handbooks and other references. These values, given by Gifford and Hanna (1970), are listed in Table 5.

TABLE 5

Values of a and b in $\sigma_z = a\ x^b$
for Area Sources

Atmospheric Stability Class	a	b
A = 1	0.4	0.91
B = 2	0.4	0.91
C = 3	0.33	0.86
DD = 4	0.22	0.80
DN = 5	0.15	0.75
E = 6	0.06	0.71
F = 7	0.06	0.71

The diffusion over cities is enhanced, compared with that over open country, due to the increased mechanical and thermal turbulence resulting from the larger surface roughness and great heat capacity of the cities. To simulate the increased surface turbulence over urban areas, PEM uses a so-called "decreased stability class index." The latter is obtained by decreasing the atmospheric stability class index by one, for all classes except Class A.

2.4 RECEPTORS

2.4.1 Receptor Grid

PEM calculates pollutant concentrations at each receptor in a rectilinear receptor array. A maximum of 2500 receptors may be used, with 50 columns and 50 rows. The spacing between each column and row is uniform, and is specified by the user. Receptors are located at the intersections of grid columns and rows. The grid spacing, number of columns, number of rows, and coordinates of the receptor at the southwest corner of the grid are used to define the grid.

Point and area sources need not necessarily be located within the grid boundaries. If area sources are included in the source inventory, the grid spacing should be selected so that the smallest area source is of the same size as a grid square. An area source is positioned on the grid by specifying the coordinates of its southwest corner. This corner should be located in the center of a receptor grid square, and not at a grid intersection, so that each square covered by the area source is centered on a receptor. For computations involving area sources, a calculation grid is defined with grid squares the same size as receptor grid squares, but with a receptor located in the center of each calculation grid square. For details, see Section 2.3.1.

2.4.2 Automatic Grid Selection

PEM has an optional subroutine which will automatically select a receptor grid for each scenario. The size and location of grids for different scenarios may differ since the selection of the receptor grid is based upon wind speed, wind direction, and atmospheric stability class.

Each source is examined sequentially. Two orthogonal axes are used with the origin located at the origin of the coordinate system for the point sources. The y axis is oriented in the north-south direction with positive values in the northerly direction. The x axis is oriented in the east-west direction with positive values in the easterly direction. Angle E is defined by

$$E = 90° - W$$

where W is the angle (measured relative to north) of the direction of the flow (see Fig. 4). The axes are then rotated through angle E such that the wind blows down the x axis. Negative values of E correspond to a clockwise rotation of coordinate axes; positive values correspond to a counter-clockwise rotation.

Parameters will be chosen for each scenario to define the automatic grid so as to provide good coverage by receptors near the point of maximum concentration. This point is determined using the Gaussian plume algorithms without pollutant removal or transformation mechanisms. For a point source, the downwind distance to the point of maximum concentration, x_{m2}, is thus calculated from

$$x_{max} = \left[\frac{b\ H^2}{a^2(b+d)} \right]^{1/2b} \tag{9}$$

where H is the effective source height, and a, b, d are coefficients defined in Tables 1 and 2. This expression is obtained by using the power laws, Eq. (5), for σ_y and σ_z in the equation for ground-level centerline concentration from an elevated point source, differentiating with respect to x, equating to zero, and solving for x.

Equation (9) is also used to determine x_{m1}, the point of maximum concentration using the physical stack height h_s instead of H. Then let

$$XTM(1) = XT + x_{m1}$$

$$XTM(2) = XT + x_{m2}$$

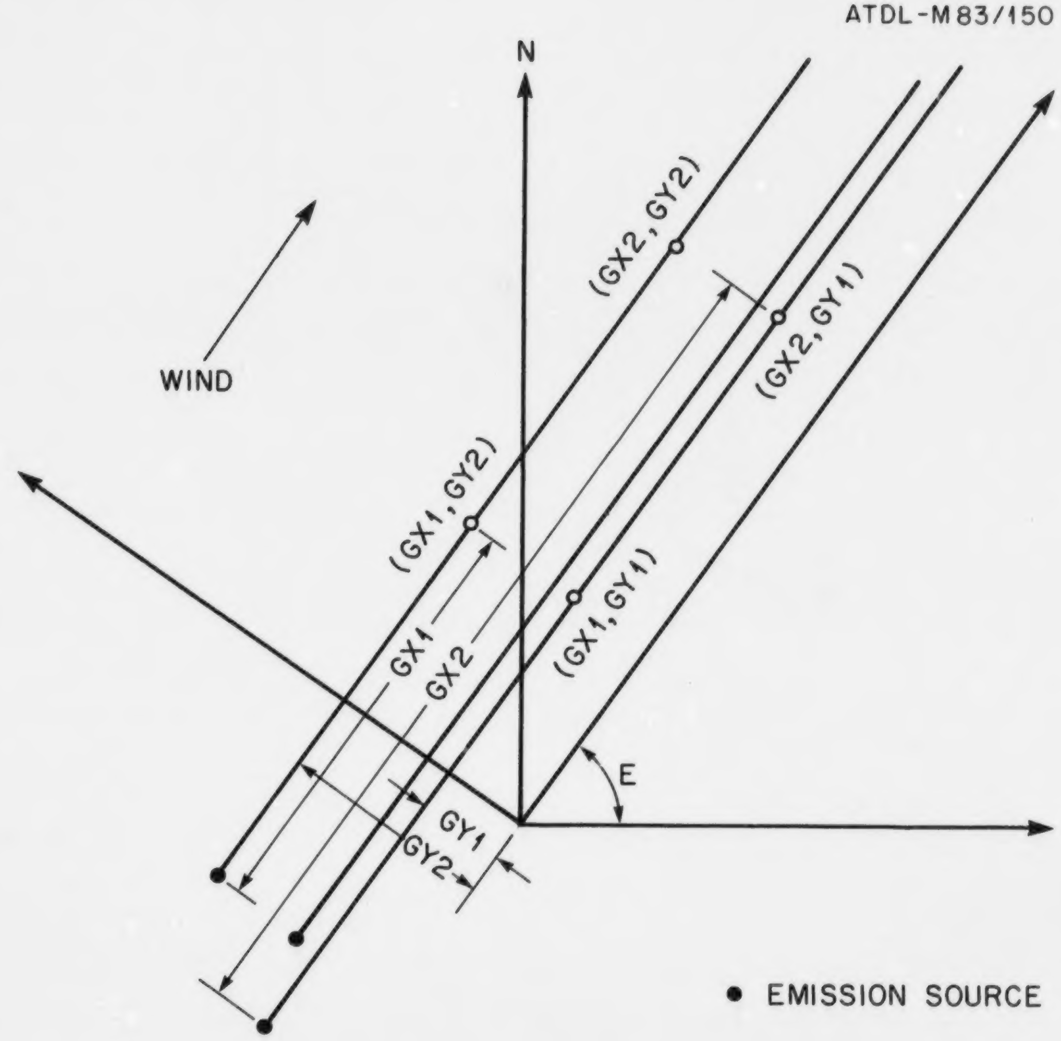

ATDL-M83/150
N
WIND
(GX2, GY2)
(GX2, GY1)
(GX1, GY2)
(GX1, GY1)
GX1
GX2
GY1
GY2
E
• EMISSION SOURCE

Figure 4. Points used for automatic selection of receptor grid by AUTGRD subroutine.

where XT is the x coordinate of the point source in the rotated coordinate system.

The largest value of XTM(2) for all point sources is GX2 and the smallest value of XTM(1) for all point sources is GX1. Let YT be the y coordinate of the point source in the rotated coordinate system. Then GY2 is the largest value of YT for all point sources and GY1 is the smallest value of YT for all point sources. These points are illustrated in Fig. 4.

Next, the points (GX1, GY1), (GX2, GY1), (GX2, GY2) and (GX1, GY2) are rotated back to the original coordinate sytem. The largest of the four x values and the largest of the four y values are chosen for the coordinates of the northeast corner of the grid. The smallest of the four x values and the smallest of the four y values are chosen for the coordinates of the southwest corner of the grid.

Then XT is defined as the distance between the x coordinates of the grid corners and YT is the distance between the y coordinates of the grid corners. Let D_{max} be the larger of XT and YT. Then D_{max} is used to determine the number of columns and rows in the receptor grid and the grid spacing. If D_{max} is larger than 10 km, then the number of rows (or columns) is 50 and the grid spacing is XT/50 (or YT/50) km. If $5 < D_{max} < 10$ km, then a grid spacing of 0.2 km is used and the number of rows (or columns) is XT/0.2 (or YT/0.2). If $0.25 < D_{max} < 5$ km, then the number of rows (or columns) is 25, and the grid spacing is $D_{max}/25$. If $D_{max} < 0.25$ km, the grid spacing is 0.01 km, the smallest possible, and the number of rows (or columns) is XT/0.01 (or YT/0.01). A typical example of the receptor grid selected by the automatic grid option is illustrated in Fig. 5.

If the culpability list option is elected in PEM, the receptor grid is limited to 25 rows and 25 columns. In this case, the grid spacing is increased so that the number of rows (or columns) does not exceed 25.

The automatic grid selection procedure, outlined above, considers only point sources. However, the chosen receptor grid may not be suitable if area sources are included in the inventory. Furthermore, the point of maximum concentration determined from Eq. (9) may be significantly in error for problems which include deposition, sedimentation, and chemical decay/transformation. The optimum receptor grid in this case should be determined by trial and error, using the receptor grid defined by this automatic grid option as the first approximation.

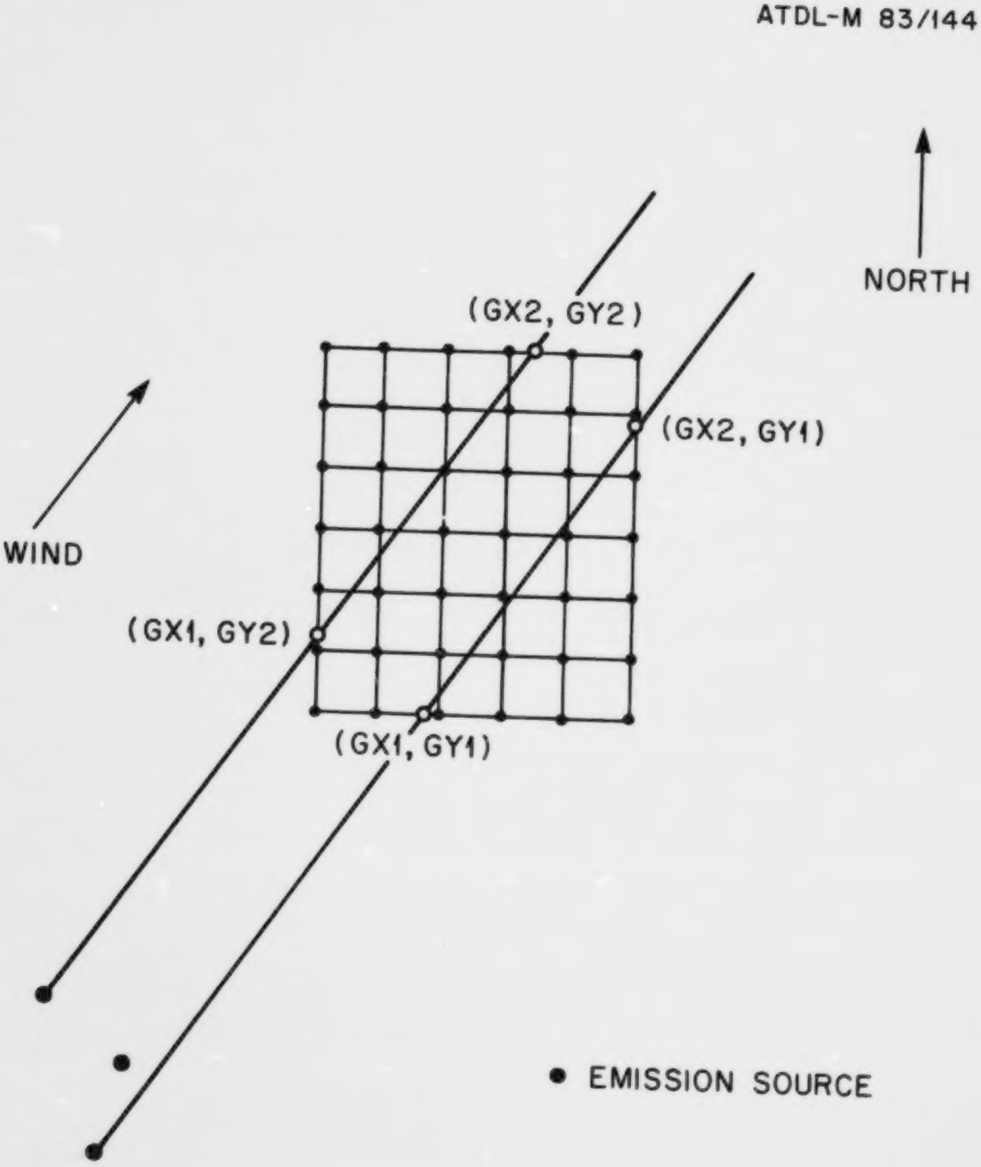

ATDL-M 83/144
NORTH
(GX2, GY2)
(GX2, GY1)
WIND
(GX1, GY2)
(GX1, GY1)
● EMISSION SOURCE

Figure 5. Example of a receptor grid selected by AUTGRD subroutine.

2.5 METEOROLOGY

The meteorological data used as input to PEM consist of the atmospheric stability class index, wind speed, wind direction, ambient temperature, mixing depth, and inversion penetration factor. This data set, which represents the mean atmospheric conditions over an hour, is called a scenario. The maximum number of scenarios in an averaging period in PEM is limited to 24, i.e., PEM is designed to predict only short-term (1 to 24 hr) average concentrations.

2.5.1 Atmospheric Stability

The Pasquill-Gifford atmospheric stability classes used in PEM are defined in Table 6.

TABLE 6

Atmospheric Stability Classes

NSC	Atmospheric Stability Class	Description
1	A	Extremely unstable
2	B	Moderately unstable
3	C	Slightly unstable
4	DD	Neutral day
5	DN	Neutral night
6	E	Slightly stable
7	F	Stable (rural only)

The relationship between the atmospheric stability classes and wind speed, incoming solar radiation, and cloud cover is given by Turner (1970) and shown below in Table 7. Class A is the most unstable, while Class F is the most stable class considered in PEM. Night refers to the period from one hour before sunset to one hour after sunrise. Note that the neutral class, D, should be assumed for overcast conditions during day or night, regardless of wind speed.

TABLE 7

Atmospheric Conditions Defining
Stability Classes (Turner, 1970)

Surface Wind Speed (at 10 meters), m/s	Day			Night	
	Incoming Solar Radiation			Thinly overcast or ≥4/8 low clouds	≤3/8 cloud
	Strong	Moderate	Slight		
<2	A	A-B	B	-	-
2-3	A-B	B	C	E	F
3-5	B	B-C	C	D	E
5-6	C	C-D	D	D	D
>6	C	D	D	D	D

2.5.2 Wind Speed

PEM gives the user the option of specifying either an hourly mean wind speed or the wind speed class number. The latter is based on National Weather Service (NWS) classification. Any wind speed which lies in a given range is assigned that class number; PEM uses a representative wind speed for each class as shown in Table 8.

TABLE 8

Wind Speed Classification

NWS Wind Speed Class	Wind Speed Range (knots)	Representative Wind Speed (m/s)
1	0 - 3	1.50
2	4 - 6	2.46
3	7 - 10	4.47
4	11 - 16	6.93
5	17 - 21	9.61
6	> 21	12.52

Wind speed near the surface generally increases with height. Most NWS wind speed measurements are taken at a height (h_o) of 10 m above the surface and are listed as "ground-level" wind speeds (U_o) in knots. Then the wind speed (U) at the physical stack height (h_s) is determined as follows:

$$U = U_o \, (h_s/h_o)^p \tag{10}$$

The wind speed U is used in the plume rise calculations and the concentration algorithms of PEM. Equation (10) is applied when the stack height is greater than 10 m. The exponent p is a function of atmospheric stability as shown in Table 9.

TABLE 9

Values of Exponent p in Wind Speed Power Law
(DeMarrais, 1959)

Atmospheric Stability Class	p
A = 1	0.10
B = 2	0.15
C = 3	0.20
DD = 4	0.25
DN = 5	0.25
E = 6	0.30
F = 7	0.30

2.5.3 Wind Direction

By convention, wind direction is defined as the direction from which the wind is blowing. PEM gives the user the option of specifying either an hourly mean wind direction, or the wind direction sector number based on the standard 16-point compass. Wind blowing from any angle in a 22.5° sector is assigned the number of that wind direction sector, and the wind direction is represented in the calculations by the median of that sector, as shown in Table 10.

TABLE 10

Wind Direction Sectors

Sector Number	Compass Point	Representative Wind Direction (deg)
1	N	0.0
2	NNE	22.5
3	NE	45.0
4	ENE	67.5
5	E	90.0
6	ESE	112.5
7	SE	135.0
8	SSE	157.5
9	S	180.0
10	SSW	202.5
11	SW	225.0
12	WSW	247.5
13	W	270.0
14	WNW	292.5
15	NW	315.0
16	NNW	337.5

PEM also includes an option in which the user specifies the wind direction in degrees for the first of four sub-scenarios; for each succeeding sub-scenario, the wind direction is automatically shifted clockwise by 90, 45, 30, 15, 10, or 5 degrees, depending on the option number specified in the input. Details of these I/O control paramters are discussed in Section 4.2.1.

2.5.4 Mixing Depth

The turbulent mixing layer near the ground is frequently bounded by a layer of stable air aloft. The latter effectively limits vertical dispersion to the mixing layer. The height of the base of the inversion above the ground is called the mixing depth, L. The hourly mixing depths are specified in the input to PEM.

If vertical mixing is limited, pollutants emitted from a point source into the mixing layer will be trapped and, beyond some point downwind, will become uniformly mixed in the vertical. PEM uses different sets of concentration algorithms for the (near-source) mixing region and the well-mixed region. The concentrations in the intermediate plume-trapping region are then obtained by interpolation as described in Section 2.2.1. The determination of the mixing regime and the algorithms to be used in the model depend on the atmospheric stability class, mixing depth, effective height of the source, and the downwind distance.

If the physical stack height exceeds the mixing depth, pollutants are emitted into the stable layer aloft; these pollutants will not be brought to the ground level and the source is neglected.

If the physical stack height is less than the mixing depth, but the effective source height (H) exceeds L, then the plume may or may not escape the mixing layer, depending on the value of H - L and the strength of the inversion. A strong inversion layer can retard the plume rise, causing the plume to be trapped in the mixing layer. PEM simulates inversions of various strengths by defining an inversion penetration factor, I. This is an optional user-specified input parameter with a default value of 2.0. The weakest inversion uses $I = 1$. If $H > I \cdot L$, then it is assumed that the plume escapes the mixing layer and the source is neglected. If $L < H \leqq I \cdot L$, then it is assumed that the plume is trapped within the mixing layer and H is set equal to L. Though somewhat crude, this procedure allows the user to account for the strength of the inversion and to obtain conservative estimates of concentrations.

SECTION 3

COMPUTER PROGRAM OVERVIEW

3.1 BASIS FOR PEM PROGRAM

The PEM (Version 82360) computer program, listed in Appendix F, is based on the FORTRAN program of the Texas Episodic Model Version 8 (TEM-8) and its Users' Guide published by the Texas Air Control Board (1979). The latter model uses the Gaussian plume concentration algorithms developed for non-reactive pollutants and a perfectly reflecting lower boundary. Chemical and physical depletion processes are therefore ignored, except for an option which allows a simple exponential decay of pollutant with travel time. This method requires an accurate estimate of the pollutant's half-life.

In contrast, PEM explicitly accounts for the dry deposition, gravitational settling, and a first-order transformation of two chemically-coupled gaseous or particulate (any size) pollutants in the concentration algorithms. The latter were developed especially for PEM by Rao (1982). The surface concentrations and deposition fluxes of both the primary pollutant (species-1 or reactant) as well as the secondary pollutant (species-2 or reaction product) are calculated. Thus, the concentration algorithms used in PEM and TEM-8 are different, though both models share essentially the same framework for calculations. Figures 2, 4, 5 and several tables shown in this report are reproduced from TEM Users' Guide with permission from Texas Air Control Board (TACB).

There are several other important differences between PEM and TEM-8. These are briefly listed below:

1. PEM uses standard EPA values for 1-hour average dispersion parameters for point sources. These correspond to the values of the 10-minute average dispersion parameters used in TEM.

2. For averaging periods longer than 10 minutes, TEM-8 uses a power law to adjust the values of σ_y to account for the greater horizontal plume meander due to fluctuations in wind direction. This is not done in PEM, since its σ_y values are assumed to represent 1-hour average dispersion of the plume.

3. TEM has eight averaging time options (NTOPT), whereas PEM has only three, namely, 1-hour, 24-hour, and N-hour ($1 < N < 24$) averaging options.

4. TEM uses the area-source algorithms given by Gifford and Hanna (1970) to calculate ground-level concentrations. The area-source algorithms used in PEM are derived by Rao (1982) from an innovative alternate approach based on mass balance considerations. These efficient new algorithms do not require additional subroutines in the program.

5. TEM uses the fast numerical technique of Christiansen and Porter (1975) in which the horizontal and vertical diffusion functions in the equation for relative concentration from a point souce are precalculated for selected values of model parameters, and stored in large arrays. For multiple sources and receptors, this technique considerably reduces the computation times required by the model, at the expense of some accuracy. Because of the large number of model parameters, PEM does not use this tabular data technique in calculations.

6. In TEM, input data can be specified in metric or British units. PEM uses only metric units.

3.2 STRUCTURE OF THE PROGRAM

Figure 6 shows the structure of PEM computer program, its subroutines and functions. All input data to the model is read through subroutine

```
           | MAIN
           |
           |
           |----- INMOD
           |
|----------+ Loop on scenarios
|          |
|          |----- INMOD
|          |
|          |----- AUTGRD ----- RISE
|          |
|          |
|    |-----+ Loop on area sources
|    |     |
|    |     |----- PSG4P ----- D01AJF ----- FUN2
|    |     |
|    |     |----- D01AJF ----- FUN3 ----- ARGCHK
|    |-----+
|          |
|          |
|    |-----+ Loop on point sources
|    |     |
|    |     |----- RISE
|    |     |
|    |     |----- QZCAL -----| RISE
|    |     |                 | EXPO
|    |     |                 | ARGCHK
|    |     |                 | PSG4P ----- D01AJF ----- FUN2
|    |     |                 | D01AJF ----- FUN1 ----- ARGCHK
|    |     |                                           EXPO
|    |     |
|    |-----+
|          |
|          |----- WORST
|          |
|          |----- WOROUT
|          |
|          |----- OUTMOD -----| WOROUT
|          |                  | ARRAY
|          |                  | SCENMX
|          |
|----------+
           |
           |----- MAXOUT
           |
```

Figure 6.   Structure of PEM computer program.

INMOD. For area source concentrations, the main program calls subroutines PSG4P (to calculate g'_{41} and g'_{42}) and D01AJF. The latter is a general purpose integration routine which calculates the integral of a function over a finite interval. After area source calculations are completed, the program starts point source calculations by calling subroutines RISE and QZCAL. The latter calculates the probability densities of vertical distributions of concentrations of the two pollutants using the appropriate algorithms. All output is printed in subroutine OUTMOD, which calls and uses other optional output routines. This procedure is repeated for all scenarios.

3.3 GENERAL FLOW OF THE PROGRAM

At the beginning of the run, PEM reads in all input data, screens them, prints warning messages, and sets default values as necessary. All control parameters are listed and explained. Input data for meteorological conditions, area sources, and point sources are also listed. Some errors in input data may be serious enough to cause cancellation of the run; however, in general, PEM attempts to recover from input errors and complete the run using default values.

Inventories of area and point sources must include the locations of the sources on a receptor grid, their emission rates, the size for area sources, and stack parameters for point sources.

The inventories are used with sets of hourly meteorological data called scenarios. For each scenario, the concentration and surface deposition flux are calculated at each impacted receptor in the grid.

Output options are many and varied. Concentration and surface deposition flux may be presented in the form of lists, array maps, and records on tape. Other options include a culpability list of point sources, a list of receptors with the highest concentration for each pollutant for each scenario, and information on plume rise and effective stack height for point sources. The calculation of the surface deposition fluxes of the species is discussed in Appendix C.

SECTION 4

PROGRAM USER'S GUIDE

4.1 SUMMARY OF PROGRAM INPUT

Control Parameters (6 cards)

Control parameters remain constant throughout the run. They specify 1) a title; 2) options for time averaging, types of input and output, and use of the stack-tip downwash algorithm; 3) receptor grid coordinates and spacing; 4) pollutant parameters and an option to calculate chemical transformation or decay; 5) scaling factors for area source emissions and calibration coefficients to be applied to the calculated concentration; and 6) labels for the pollutants and calibration coefficients.

Scenario Parameters (1-24 cards)

Each card contains information for one scenario, that is, the meteorological data for one hour. It includes atmospheric stability class, wind speed, wind direction, temperature, the inversion penetration factor, and mixing height.

Area Source Parameters (0-50 cards)

Each card contains information for one area source. It includes the location of the area source on the receptor grid, the size of the area source, and its emission rates.

A blank card must follow the last area source card to signal the end of the area source data.

Point Source Parameters (0-300 cards)

Each card contains information for one point source. It includes the location of the point source on the receptor grid; its emission rates; the stack parameters of height, diameter, exit velocity, and exit temperature; and a label which identifies the point source.

A blank card must follow the last point source card to signal the end of the point source data.

4.2 DETAILS OF PROGRAM INPUT

4.2.1 Control Parameters (6 cards)

Card 1 : Title FORMAT(20A4)

Alphanumeric information which identifies the run. The information is printed at the top of each page of output.

Card 2 : Input and output options FORMAT(13I5)

NTOPT Averaging time option
In PEM, a scenario is a set of meteorological data for one hour.
=1 One hour: Concentrations are calculated for each scenario. No averaging is done.
=2 Twenty-four hours: Concentrations are calculated for exactly 24 scenarios and averaged.
=3 Variable: Concentrations are calculated for a given number of scenarios (2 to 24) and averaged.
The default value is NTOPT=1 .

NWDOPT Wind direction input option
=0 The user will specify wind direction in degrees for each scenario.
=1 The user will specify a wind direction sector number for each scenario.
=2-7 The user will specify wind direction in degrees for the first of four sub-scenarios. For each succeeding sub-scenario, the wind direction is automatically shifted clockwise by 90,45,30,15,10, or 5 degrees, depending on the option number selected.
NWDOPT= 2-7 is not allowed with time averaging (NTOPT=2 or 3).
The default value is NWDOPT=0 .

NWSOPT Wind speed input option
Surface wind speed is measured at 10 meters.
=0 The user will specify surface wind speed in meters/second for each scenario.
=1 The user will specify a wind speed class number for each scenario.
The default value is NWSOPT=0 .

NSCEN Number of scenarios
=1-24 The number of sets of one-hour meteorological data to be read and processed by the program. When the time-averaging option NTOPT=2, NSCEN must equal 24 . If NSCEN is not specified properly, the input data file will be misread.
The default value is NSCEN=1 .

NLIST Output option for lists of calculated concentration and surface deposition flux at each receptor in the grid.

=0 The lists are not printed.

=1 Lists of concentration and surface deposition flux are printed, one column of the grid per page.

The default value is NLIST=0 .

NLIST=1 may not be used with the automatic windshift option (NWDOPT>1) .

NARRAY Output option for array maps of calculated concentration and surface deposition flux at each receptor in the grid.

=0 No array maps are printed.

=1 Separate maps of uncalibrated and calibrated concentration and surface deposition flux are printed--a total of four maps for each pollutant.

=2 Maps of uncalibrated values only are printed --two maps for each pollutant.

=3 Maps of calibrated values only are printed --two maps for each pollutant.

The default value is NARRAY=0 .

NTAPE Output option for a list on tape of concentration and surface deposition flux at each receptor in the grid.

=0 The list is not written to tape.

=1 A list of concentration and surface deposition flux is written on a separate output tape, one receptor per record. Control parameter INTER may be set to limit the number of receptors written onto tape. The program checks the total number of records to be written; if the number is greater than 10,000 a message is printed and NTAPE is set to zero.

The default value is NTAPE=0 .

NTAPE=1 may not be used with the automatic windshift option (NWDOPT>1) .

NCSOPT Output option for a culpability list of the five point sources which contribute most to the total concentration calculated at each receptor.

=0 The culpability list is not printed.

=1 For each receptor in the grid, the program lists up to five point sources and the percent of the total concentration contributed by each source. The total concentration and surface deposition flux at each receptor are also listed. The information is printed one column of the grid per page.

The default value is NCSOPT=0 .

NCSOPT=1 may not be used when two pollutants are specified (NPOL=2) , or when the number of columns in the grid (LX) or the number of rows in the grid (LY) is greater than 25 .

NMAX	Output option for lists of the maximum concentration and surface deposition flux calculated for each pollutant for each scenario.
=0	The lists are not printed.
=1	At the end of the run, lists are printed to show the receptor in each scenario which received the highest concentration and surface deposition flux for each pollutant.
	The default value is NMAX=0 .
NSTDWN	Option for point source stack-tip downwash algorithm
=0	The stack-tip downwash algorithm is used to determine stack-tip downwash effects for point sources.
=1	The algorithm is not used.
	Note that the default value NSTDWN=0 means the algorithm is used.
INTER	Interval option for receptors written to tape
=N	When the output option NTAPE=1 is selected, the value of INTER determines which receptors are written on the tape. When INTER is specified as integer N, every Nth receptor in each column and row is listed. Thus, if INTER = 2, one fourth of the receptors will be listed ; if INTER is 5, one twenty-fifth will be listed. Effectively, an output grid is set up with spacing equal to the value of INTER, and only those receptors on the "new" grid are written onto the tape.
	The default value is INTER=1 ; that is, every receptor in the grid will be listed on the tape.
	INTER is used only when output option NTAPE=1 is selected.
NPRINT	Output option for point source information
= 0	Input point source data is printed only at the beginning of the run.
= 1	A list of input point source parameters and calculated plume rise information is printed at the beginning of each scenario.
	The default value is NPRINT=0 .

INPTSC Input option for point source data
= 1 Point source data is read from the normal input stream (on cards, for example).
= 2 Point source data is read from a disk file specified by the user in his job control set.
The default value is INPTSC=1 .

Card 3 : Grid information FORMAT (2F10.0,2I10,3F10.0)

XRSWC The x, or east-west coordinate of the receptor at the southwest corner of the grid, in kilometers.
The default value is XRSWC=0.0 km.

YRSWC The y, or north-south coordinate of the receptor at the southwest corner of the grid, in kilometers.
The default value is YRSWC=0.0 km.

LX The number of columns of receptors in the receptor grid.
Allowable values are 1 to 50 .
The default value is LX=1 .

LY The number of rows of receptors in the receptor grid.
Allowable values are 1 to 50 .
The default value is LY=1 .

GRID Automatic grid option or grid spacing
=0.0 The program chooses the size and placement of the receptor grid to insure that the point of maximum concentration calculated from point sources will fall within the grid. Note that area sources are not taken into consideration in this selection.
≠0.0 The size of the spacing between columns and rows of receptors in the grid, in kilometers.
The default value is GRID=0.0 km., the automatic grid selection.

DTDZ(1), DTDZ(2) The potential temperature gradient, $d\theta/dz$, for Class E and Class F atmospheric stability, in units of degrees Celsius/meter.
The potential temperature gradient is used in the stable/buoyant and stable/momentum plume rise equations.
The default values are DTDZ(1)=0.02 deg C/meter and DTDZ(2)=0.035 deg C/meter.

Card 4 : Pollutant information and calculation option
FORMAT(2I5,6F10.0)

NPOL	The number of pollutants Allowable values are 1 or 2 . The default value is NPOL=1 .
ICT	Option to calculate chemical transformation or decay
=0	Chemical transformation loss of pollutant(s) is not considered.
=1	When NPOL=1, the first-order chemical decay of the pollutant is considered. When NPOL=2, the first-order chemical transformation of pollutant-1 to pollutant-2 is considered. The default value is ICT=0 .
VD1	Deposition velocity for pollutant-1, in cm/second When area source calculations are included, VD1 should not be zero.
W1	Settling velocity for pollutant-1, in cm/second
VD2	Deposition velocity for pollutant-2, in cm/second. When NPOL=2 and area source calculations are included, VD2 should not be zero.
W2	Settling velocity for pollutant-2, in cm/second

In general, for deposition to occur, the settling velocity (W) should be less than or equal to the deposition velocity (VD). For gases and very small particles, W should be zero. For small particles, W should be less than VD. For medium and large particles, W should equal VD.

XKT	Chemical transformation or decay rate of pollutant-1, in percent/hour. Allowable values are 0.1 to 100.0 percent/hour; input values outside that range are set to the nearer limit. For example, if XKT=0.0 is specified, the program prints a message and sets XKT=0.1 percent/hr. XKT is used only when option ICT=1 is selected.
GAMMA	The ratio of the molecular weights of pollutant-2 (product) to pollutant-1 (reactant) in the chemical transformation. GAMMA is used only when option ICT=1 is selected. The default value is GAMMA=0.0 .

Card 5 : Scaling and calibration   FORMAT(6F10.0)

ASCALE(1), ASCALE(2) Area source scaling factors for pollutants 1 and 2 .
All area source emission rates are multiplied by ASCALE(1) for pollutant-1 and by ASCALE(2) for pollutant-2 .
The default values are ASCALE(1)=1.0 and ASCALE(2)=1.0 .

The entire area source inventory can be scaled to reflect higher traffic volume, etc. in future years, without having to generate an entire new set of area sources.

A(1), B(1) Coefficients used to calibrate the calculated concentration of pollutant-1.
The calibrated value Xcal is computed by applying A and B to the concentration X by the formula

$$Xcal = A + BX$$

The default values are A(1)=0.0 and B(1)=0.0 .

A(2), B(2) Coefficients used to calibrate the calculated concentration of pollutant-2.
The default values are A(2)=0.0 and B(2)=0.0 .

The normal output units for calculated concentration are micrograms per cubic meter. The calibration coefficients can be used to convert to percent allowable , parts per million, or any other convenient units.

Card 6 : Labels   FORMAT (3A4,7A4,3A4,7A4)

POLNAM(1) Name for pollutant-1
Up to 12 alphanumeric characters are allowed.

CALNAM(1) Label for calibrated values of concentration of pollutant-1, computed from calibration coefficients A(1) and B(1) on Card 5.
Up to 28 alphanumeric characters are allowed.

POLNAM(2) Name for pollutant-2
Up to 12 alphanumeric characters are allowed.

CALNAM(2) Label for calibrated values of concentration of pollutant-2, computed from calibration coefficients A(2) and B(2) on Card 5.
Up to 28 alphanumeric characters are allowed.

Defaults for all labels are blanks.

4.2.2 Scenario Parameters FORMAT(3I5,5F10.0)

One to 24 cards, each containing a set of meteorological data for one hour.

NSC	Atmospheric stability class number Allowable values are 1 through 7; an input value outside that range will be set to the nearer limit. See List of Tables for atmospheric stability classes used in PEM.
NWS	Wind speed class Allowable values are 1 through 6; an input value outside that range will be set to the nearer limit. See List of Tables for wind speed classes used in PEM. Note that NWS is used only when the windspeed input option NWSOPT on Card 2 is specified as NWSOPT=1 .
NWD	Wind direction sector Allowable values are 1 through 16; any input value outside that range will be set to the nearer limit. See List of Tables for wind direction sectors used in PEM. Note that NWD is used only when the wind direction option NWDOPT on Card 2 is specified as NWDOPT=1 .
WS	Wind speed Surface wind speed in meters/second measured at a height of ten meters. If WS=0.0 is specified, a message is printed and WS is set to 1.0 m/sec. Note that WS is used only when the wind speed input option NWSOPT on Card 2 is specified as NWSOPT=0 .
WD	Wind direction The azimuthal angle in degrees from which the wind is blowing. Allowable values are 0.0 through 360.0 degrees. The default value is WD=0.0 , wind from the north. Note that WD is used only when the wind direction input option NWDOPT on Card 2 is specified as NWDOPT=0 or 2 through 7 .
TA	Ambient temperature in degrees Celsius. The default value is TA=0.0 deg C.

PEN Inversion penetration factor
When the top of a stack is below the mixing height, but the calculated effective stack height is greater than the mixing height, the inversion penetration factor is used to determine whether the plume can penetrate the upper level inversion boundary .
Values for PEN can range from 1.0 for a weak inversion to 2.0 or more for a strong inversion.
The default value is PEN=2.0 .

HMIX Mixing height
The distance in meters from the ground to the bottom of a layer of stable air.
The default value is HMIX=9999.99 m.

4.2.3 Area Source Parameters FORMAT(5F10.0)

Zero to 50 cards, each containing parameters for one area source. A blank card must follow the last area source data card.

XA The x, or east-west, coordinate of the south-west corner of the area source, in kilometers.
The default value is XA=0.0 km.

YA The y, or north-south, coordinate of the south-west corner of the area source, in kilometers.
The default value is YA=0.0 km.

SIZE The length of a side of the area source, in meters.
The default value is SIZE=GRID*1000.0, the size of one grid square in meters. If GRID is specified as zero, then SIZE is set to 1.0E-4 meters.

EA(1), EA(2) Emission rates for pollutants 1 and 2 in grams/second.
Note that this is not an emission rate per unit area; this is the emission rate of an equivalent point source located at the center of the area source.
The default values are EA(1)=0.0 g/sec and EA(2)=0.0 g/sec.

Note: The area source inventory is followed by a blank card to signal the end of area source data.

4.2.4 Point Source Parameters FORMAT(8F9.0,2A4)

Zero to 300 cards, each containing parameters for one point source. A blank card must follow the last point source data card.

XP The x, or east-west, coordinate of the point source, in kilometers.
The default value is XP=0.0 km.

YP The y, or north-south, coordinate of the point source, in kilometers.
The default value is YP=0.0 km.

EP(1), EP(2) Emission rates for pollutants 1 and 2 in grams/second.
The default values are EP(1)=0.0 g/sec and EP(2)=0.0 g/sec.

HP The physical height of the stack, in meters.
The default value is HP=0.0 m.

DP The inside exit diameter of the stack, in meters. If DP=0.0 is specified, a message is printed and DP is set to 1.0E-4 meters.

VP The stack-exit velocity of the plume, in meters/second.
The default value is VP=0.0 meters/sec, which will yield zero plume rise.

TP The stack-exit temperature of the plume, in degrees Celsius.
The default value is TP=0.0 deg C, which usually results in a momentum-dominated plume rise.

NAME Label which identifies the point source. Up to eight alphanumeric characters may be used.
The default is blanks.

Note: The point source inventory is followed by a blank card to signal the end of the point source data.

4.2.5 Discussion of Input Parameters

The PEM, designed to predict short-term (1 to 24 hr) average ground-level concentrations, assumes that emission rates are constant over the averaging period for NTOPT > 1. This may not be a good assumption for cases where the emissions are strongly time-dependent. For these cases, concentration estimates may be made for each hour using the appropriate emissions and the mean meteorological conditions for that hour. Then concentrations for a period longer than an hour can be determined by averaging the hourly concentrations of that period. This can be done externally with minimal programming.

The deposition and sedimentation velocities of the species and the chemical transformation rate are also assumed to be constant over the concentration-averaging period. If it is important to consider the hourly variations of these parameters, a procedure similar to that described above for emissions, can be used in the concentration calculations.

The meteorological data input to PEM consist of atmospheric stability class, wind speed, wind direction, temperature, the inversion penetration factor, and mixing height. Each of these hourly data sets is called a scenario. For a given set-up of the receptor grid, the pattern of the impacted receptors downwind of a source depends primarily on the wind direction. For urban-planning or regulatory purposes, it may be necessary to investigate the effects of different wind directions on the calculated concentration patterns in the receptor grid. The PEM has an option which divides each scenario into four sub-scenarios, each consisting of the same hourly meteorological data except for the wind direction. When the user selects this automatic windshift option (i.e., NWDOPT > 1), the wind direction for only the first of the four sub-scenarios is specified by the user. For each succeeding sub-scenario, the wind direction is automatically shifted clockwise by a fixed number of degrees and the concentration calculations are repeated. The magnitude of this shift may be as large as 90° (for NWDOPT = 2), or as small as 5° (for NWDOPT = 7).

The calculated concentrations, C_i, of the species in the PEM are given in $\mu g/m^3$; these are referred to as uncalibrated values, and represent only the contributions of the sources to the concentrations at the receptors. The user may add the background concentrations, or express the calculated concentrations in parts per million or percent allowable, by the formula

$$C_i^* = A_i + B_i \cdot C_i \ , \quad i = 1 \text{ or } 2,$$

where A_i and B_i are the user-specified calibration coefficients (with default values of zero), and C_i^* are the calibrated concentrations of the species. Depending on the value specified for NARRAY, the PEM output may consist of array maps of either uncalibrated values or calibrated values, or both, of concentrations and surface deposition fluxes.

The culpability list output option, NCSOPT, is used for evaluation of control strategies. When this option is in effect, the five point sources which contributed most to the total concentration at each receptor are identified and their percent contributions are printed for each scenario. This option may be used only when the model calculates concentrations of a single pollutant (NPOL = 1).

Based on the number of pollutants (NPOL = 1 or 2) and the chemical transformation/decay option parameter (ICT = 0 or 1) specified in the input to the model, PEM program does one of the following:

(1) If NPOL = 1 and ICT = 0 or 1, surface concentrations and deposition fluxes of one gaseous or particulate pollutant, with the given deposition and settling velocities, VD1 and W1 respectively, are calculated. If ICT = 1, then chemical decay of the pollutant is also considered if the decay rate XKT > 0. is given.

(2) If NPOL = 2 and ICT = 0, surface concentrations and deposition fluxes of two different and uncoupled gaseous or particulate pollutant species with the given deposition and settling velocities, VD1 and W1 (for species-1) and VD2 and W2 (for species-2) respectively, are calculated. Emission rates for both species may be different. Chemical decay is not considered for either species even if XKT > 0.

(3) If NPOL = 2 and ICT = 1, the two gaseous or particulate pollutant species are coupled through a first-order chemical transformation. The surface concentrations and deposition fluxes of both the primary pollutant (species-1 or reactant) as well as the secondary pollutant (species-2 or reaction product) are calculated. The chemical transformation rate (XKT > 0.) should be given. Non-zero direct emissions of the secondary pollutant from the point and/or area sources may also be specified as input for this case.

In the expressions for concentrations from area sources, Eq. (8), the parameter V_{d1} and V_{d2} should be non-zero to avoid singularities in the computations. If either one of these parameters is input as zero, PEM uses a default value of 0.01 cm/s when area sources are included in the emission inventory. The specification of the deposition and gravitational settling velocities in the model is discussed in Appendix C.

4.3 GUIDE TO PROGRAM OUTPUT

At the beginning of each scenario or sub-scenario*:

NPRINT---Point source parameter list

For each point source, the output lists its coordinates on receptor grid, emission rates, stack parameters, dominant influence of plume rise, wind speed at physical stack height, and maximum effective source height.

At the end of each scenario or sub-scenario:

NCSOPT---Point source culpability list

For each receptor in the grid, the five point sources which contributed most to the total concentration at the receptor are identified. For each receptor, the output includes the five point source sequence numbers, the percent of the total concentration each of the five produced, and the total concentration and surface deposition flux at the receptor. The information is printed one column of the grid per page. To reduce the amount of output produced, only columns containing non-zero concentrations are printed.

NLIST---Concentration and surface deposition flux list

For each receptor in the grid, the calculated concentration and surface deposition flux are listed, one column of the grid per page. To reduce the amount of output produced, only columns containing non-zero concentrations are printed.

NTAPE---Concentration and surface deposition flux tape

The calculated concentration and surface deposition flux at each receptor on the grid are written onto a separate output tape. All records on the tape contain eighty alphanumeric characters. A separate record is written for every receptor in the grid, unless the interval parameter INTER has been specified as greater than one.
The first record on the tape contains the title information given on Card 1 of the Control Parameter cards, written by FORMAT(20A4). Succeeding records contain the x,y coordinates of the receptor; values for concentration,

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*When the automatic windshift option is selected (NWDOPT>1), a scenario is divided into four sub-scenarios, each with a different wind direction.

surface deposition flux, calibrated concentration, and calibrated surface deposition flux for pollutant-1; and values for concentration, surface deposition flux, calibrated concentration, and calibrated surface deposition flux for pollutant-2. These values are written by FORMAT(10F8.2).

NARRAY---Array maps of concentration and surface deposition flux

Separate maps are printed for concentration and surface deposition flux for each pollutant. The concentration or surface deposition flux at each receptor is printed at its relative location on the grid to aid in visualization of the distribution of the pollutant.
The value specified for NARRAY determines which maps are printed. If output for both uncalibrated and calibrated values is chosen, four maps will be produced for each pollutant. If output is chosen for only uncalibrated, or only calibrated, values, two maps will result for each pollutant. Each map can require one, two, or four pages of output to display the entire grid, since each page can display values for up to 25 grid columns and 25 grid rows.

At the end of the run:

NMAX---Maximum concentration and surface deposition flux

For each scenario, the receptor which receives the highest concentration of pollutant-1 and the receptor which receives the highest concentration of pollutant-2, and the concentration at each, are listed. A second list gives the surface deposition flux at these receptors.

When time averaging is selected (NTOPT=2 or 3), NCSOPT output is printed after each scenario, but output for NLIST, NTAPE, and NARRAY is printed only after all scenarios have been processed, and only for the averaged time.

4.4 EXAMPLE PROBLEMS

Three example runs are described here and their results shown in Appendix E to demonstrate the use of the PEM program.

Example 1

Pollutant-1 is a gas, and pollutant-2 is made of small particles which deposit on the ground without significant settling ($V_d > 0$ and $W = 0$). This example uses an area source and two point sources on a finely-spaced receptor grid. Chemical transformation is selected with a transformation rate of one percent/hour; however, the relatively high emission rates chosen for pollutant-2 probably contribute most to its concentration. The example is a simple one, with no time averaging and only one scenario. Wind speed class number and wind direction sector number are specified. The output options selected print point source plume rise information, concentration and surface deposition flux array maps, and the receptor with the highest concentration.

Example 2

This example demonstrates the chemical transformation of a gaseous pollutant to a small-particulate pollutant whose deposition is due primarily to non-gravitational effects ($V_d > W > 0$). A fast transformation rate of twenty percent/hour is specified. Concentrations contributed by multiple point and area sources are calculated and averaged over three hours with the meteorological data held constant. Array maps of concentration and surface deposition flux and the receptor with the highest concentration are printed.

Example 3

A gaseous pollutant and a large-particulate pollutant are modeled, using one large area source and three point sources on a widely-spaced receptor grid. In this example, point source emission rates for pollutant-2 are specified as zero. Under this condition, the chemical transformation of pollutant-1, at a rate of ten percent/hour, accounts for all of the pollutant-2 concentration produced by the point sources. Concentrations are averaged over six hours of slightly varying meteorological data. The general atmospheric conditions are slightly stable, with relatively cool temperatures and low mixing heights; low wind speeds and constant wind direction are specified in meters/second and degrees, respectively. The output includes point source plume rise information for each scenario, array maps of concentration and surface deposition flux, and the receptor with the highest concentration in each of the six scenarios.

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APPENDIX A

POINT SOURCE ALGORITHMS

The algorithms used in PEM to calculate ground-level concentrations of gaseous or particulate pollutants released from an elevated continuous point source are derived by Rao (1982). These algorithms are based on a gradient-transfer model which describes the atmospheric transport, diffusion, dry deposition, sedimentation, and a first-order chemical transformation of pollutants. The analytical solutions of the model are expressed in terms of the empirical Gaussian plume dispersion parameters and extended to various atmospheric stability and mixing conditions. Details of the model and the solutions can be found in that reference. Here we only list the parameterized point source algorithms for the primary (reactant) and the secondary (reaction product) pollutants, denoted by subscripts 1 and 2, respectively.

For convenience, we adopt the following nondimensionalization scheme: All velocities are nondimensionalized by U, the constant mean wind speed. The horizontal downwind distance x and all vertical height quantities are nondimensionalized by $\sqrt{2}\ \sigma_z$; the chemical transformation time scale τ_c is nondimensionalized by $\sqrt{2}\ \sigma_z/U$. The horizontal crosswind distance y is nondimensionalized by $\sqrt{2}\ \sigma_y$. Thus, we define

$$
\begin{aligned}
&\hat{V}_{d1} = V_{d1}/U \quad , \quad \hat{V}_{d2} = V_{d2}/U \\
&\hat{W}_1 = W_1/U \quad , \quad \hat{W}_2 = W_2/U \\
&\hat{V}_{11} = \hat{V}_{d1} - \hat{W}_1/2 \quad , \quad \hat{V}_{12} = \hat{V}_{d2} - \hat{W}_2/2 \\
&\hat{V}_{13} = \hat{V}_{11} - (\hat{W}_1 - \hat{W}_2)/2 \\
&\hat{V}_{21} = \hat{V}_{d1} - \hat{W}_1 \quad , \quad \hat{V}_{22} = \hat{V}_{d2} - \hat{W}_2 \\
&\hat{x} = x/\sqrt{2}\,\sigma_z \quad , \quad \hat{z} = z/\sqrt{2}\,\sigma_z \\
&\hat{H} = H/\sqrt{2}\,\sigma_z \quad , \quad \hat{L} = L/\sqrt{2}\,\sigma_z \\
&\hat{\tau}_c = \tau_c U/\sqrt{2}\,\sigma_z \quad , \quad \hat{y} = y/\sqrt{2}\,\sigma_y
\end{aligned}
\tag{A-1}
$$

where

H = effective height of source

L = height of the inversion lid or mixing depth

V_{d1} , V_{d2} = dry deposition velocities of primary and secondary pollutants

W_1 , W_2 = gravitational settling velocities of primary and secondary pollutant particles

x, y, z = horizontal downwind, horizontal crosswind, and vertical coordinates

σ_y , σ_z = Gaussian dispersion parameters in y and z directions

τ_c = characteristic time scale of first-order chemical transformation.

The nondimensional functions g'_{21} and g'_{22} used in Eq. (1) of Section 2.2.1 are now defined as follows:

$$g_1(\hat{x},\hat{y}) = \exp(-\,\hat{y}^2) \tag{A-2}$$

$$g'_{21}(\hat{x},0) = \exp(-\beta_1^2 - \hat{H}^2 - \hat{x}/\hat{t}_c)\cdot(2 - \alpha_1) \tag{A-3}$$

where $$\beta_1^2 = -\,2\,\hat{W}_1\,\hat{x}\,\hat{H} + \hat{W}_1^2\,\hat{x}^2$$

$$\alpha_1 = 4\sqrt{\pi}\,\hat{V}_{11}\,\hat{x}\;\;e^{\xi_1^2}\,\mathrm{erfc}\;\xi_1 \tag{A-4}$$

$$\xi_1 = \hat{H} + 2\,\hat{V}_{11}\,\hat{x}$$

$$\begin{aligned} g'_{22}\,(\hat{x},0) = e^{-\beta_2^2}\Big[& (Q_2/Q_1 + \gamma)\;\; e^{-\hat{H}^2}\cdot(2 - \alpha_2) \\ & -\gamma\,\exp(-\hat{H}^2 - \hat{x}/\hat{t}_c)\cdot(2 - \alpha_3) \\ & -\gamma\,4\sqrt{\pi}\,(\hat{V}_{21} - \hat{V}_{22})\,\hat{x}\cdot F_1(\hat{x},0)\Big] \end{aligned} \tag{A-5}$$

where $$\beta_2^2 = -\,2\,\hat{W}_2\,\hat{x}\,\hat{H} + \hat{W}_2^2\,\hat{x}^2$$

$$\alpha_2 = 4\sqrt{\pi}\,\hat{V}_{12}\,\hat{x}\;\;e^{\xi_2^2}\,\mathrm{erfc}\;\xi_2$$

$$\alpha_3 = 4\sqrt{\pi}\,\hat{V}_{13}\,\hat{x}\;e^{\xi_3^2}\,\mathrm{erfc}\,\xi_3$$

$$\xi_2 = \hat{H} + 2\,\hat{V}_{12}\,\hat{x}\,, \quad \xi_3 = \hat{H} + 2\,\hat{V}_{13}\,\hat{x} \tag{A-6}$$

and

$$F_1(\hat{x},0) = \frac{1}{\pi}\int_o^1 \frac{1}{\sqrt{t(1-t)}}\;\exp\left(\frac{-\hat{H}^2}{t} - \frac{\hat{x}t}{\hat{t}_c}\right)\;.$$

$$\left[1 - \sqrt{\pi}\,(\xi_4 - \hat{H}/\sqrt{t})\;e^{\xi_4^2}\,\mathrm{erfc}\,\xi_4\right]$$

$$\left[1 - \sqrt{\pi}\,\xi_5\;e^{\xi_5^2}\;\mathrm{erfc}\,\xi_5\right]\,dt \tag{A-7}$$

where

$$\xi_4 = \hat{H}/\sqrt{t} + 2\,\hat{V}_{13}\,\hat{x}\,\sqrt{t}$$

$$\xi_5 = 2\,\hat{V}_{12}\,\hat{x}\,\sqrt{1-t} \tag{A-8}$$

In Eq. (A-5), γ is the ratio of molecular weight of the secondary pollutant to molecular weight of the primary pollutant, and Q_2/Q_1 is the corresponding ratio of emission rates of species. In Eq. (A-7), t is a dimensionless dummy variable of integration with limits of 0 and 1.

The nondimensional functions g'_{41} and g'_{42} used in Eq. (2) of Section 2.2.1 are defined as follows:

For $\hat{V}_{d1} \neq \hat{W}_1$ or $\hat{V}_{21} \neq 0$,

$$g'_{41}(\hat{x}) = \exp(-\beta_1^2 - \hat{x}/\hat{\tau}_c)\left[(\hat{V}_{11}/\hat{V}_{21})\, e^{\xi_1^2}\, \text{erfc}\, \xi_1 - (\hat{W}_1/2\hat{V}_{21})\, e^{\beta_1^2}\, \text{erfc}\, \beta_1\right] \tag{A-9}$$

where $\xi_1 = 2\,\hat{V}_{11}\,\hat{x}$ and $\beta_1 = \hat{W}_1\,\hat{x}$.

For $\hat{V}_{d1} = \hat{W}_1$ or $\hat{V}_{21} = 0$,

$$g'_{41}(\hat{x}) = \exp(-\xi_1^2 - \hat{x}/\hat{\tau}_c)\left[(1 + 2\,\xi_1^2)\, e^{\xi_1^2}\, \text{erfc}\, \xi_1 - 2\,\xi_1/\sqrt{\pi}\right] \tag{A-10}$$

where $\xi_1 = 2\,\hat{V}_{11}\,\hat{x} = \hat{V}_{d1}\,\hat{x} = \hat{W}_1\,\hat{x}$.

For $\hat{V}_{21} \neq 0$ and $\hat{V}_{22} \neq 0$,

$$\begin{aligned} g'_{42}(\hat{x}) = e^{-\beta_2^2}\Big[\ & (Q_2/Q_1 + \gamma)\left\{(\hat{V}_{12}/\hat{V}_{22})\, e^{\xi_2^2}\, \text{erfc}\, \xi_2 - (\hat{W}_2/2\hat{V}_{22})\, e^{\beta_2^2}\, \text{erfc}\, \beta_2\right\} \\ & - \gamma\, e^{-\hat{x}/\hat{\tau}_c}\left\{(\hat{V}_{13}/\hat{V}_{21})\, e^{\xi_3^2}\, \text{erfc}\, \xi_3 - (\hat{W}_2/2\,\hat{V}_{21})\, e^{\beta_2^2}\, \text{erfc}\, \beta_2\right\} \\ & - \gamma\, 4\sqrt{\pi}\,(\hat{V}_{21} - \hat{V}_{22})\,\hat{x}\cdot F_2(\hat{x})\ \Big] \end{aligned} \tag{A-11}$$

where $\xi_2 = 2\,\hat{V}_{12}\,\hat{x}\ ,\quad \beta_2 = \hat{W}_2\,\hat{x}$

$$\xi_3 = 2\,\hat{V}_{13}\,\hat{x}\ ,\quad \hat{V}_{13} = \hat{V}_{11} - (\hat{W}_1 - \hat{W}_2)/2 \tag{A-12}$$

$$F_2(\hat{x}) = \frac{1}{2\pi}\int_0^1 \frac{1}{\sqrt{t}} \exp(-\hat{x}t/\hat{\tau}_c) \left[1 - \sqrt{\pi}\, \xi_4\, e^{\xi_4^2} \operatorname{erfc} \xi_4 \right] \cdot$$

$$\left[(\hat{V}_{12}/\hat{V}_{22})\; e^{\xi_5^2} \operatorname{erfc} \xi_5 - (\hat{W}_2/2\hat{V}_{22})\; e^{\xi_6^2} \operatorname{erfc} \xi_6 \right] dt, \qquad \text{(A-13)}$$

where $\xi_4 = \xi_3 \sqrt{t}$, $\xi_5 = \xi_2 \sqrt{1-t}$, $\xi_6 = \beta_2 \sqrt{1-t}$ (A-14)

For $\hat{V}_{21} \neq 0$ and $\hat{V}_{22} = 0$,

$$g'_{42}(\hat{x}) = e^{-\xi_2^2} \Bigg[(Q_2/Q_1 + \gamma) \left\{ (1 + 2\,\xi_2^2)\, e^{\xi_2^2} \operatorname{erfc} \xi_2 - 2\,\xi_2/\sqrt{\pi} \right\}$$

$$- \gamma\, e^{-\hat{x}/\hat{\tau}_c} \left\{ (\hat{V}_{13}/\hat{V}_{21})\; e^{\xi_3^2} \operatorname{erfc} \xi_3 - (\hat{W}_2/2\hat{V}_{21})\; e^{\xi_2^2} \operatorname{erfc} \xi_2 \right\}$$

$$- \gamma\, 4\sqrt{\pi}\; \hat{V}_{21}\, \hat{x} \cdot F_2(\hat{x}) \Bigg] \qquad \text{(A-15)}$$

where $\xi_2 = 2\, \hat{V}_{12}\, \hat{x} = \hat{V}_{d2}\, \hat{x} = \hat{W}_2\, \hat{x} = \beta_2$

$\xi_3 = 2\, \hat{V}_{13}\, \hat{x}$

$$F_2(\hat{x}) = \frac{1}{2\pi}\int_0^1 \frac{1}{\sqrt{t}} \exp\,(-\hat{x}t/\hat{\tau}_c) \cdot \left[1 - \sqrt{\pi}\, \xi_4\, e^{\xi_4^2} \operatorname{erfc} \xi_4 \right] \cdot$$

$$\left[(1 + 2\,\xi_5^2)\, e^{\xi_5^2} \operatorname{erfc} \xi_5 - 2\,\xi_5/\sqrt{\pi} \right] dt, \qquad \text{(A-16)}$$

with $\xi_4 = \xi_3 \sqrt{t}$, $\xi_5 = \xi_2 \sqrt{1-t}$.

For $\hat{V}_{21} = 0$ and $\hat{V}_{22} \neq 0$,

$$g'_{42}(\hat{x}) = e^{-\xi_3^2} \Bigg[(Q_2/Q_1 + \gamma) \left\{ (\hat{V}_{12}/\hat{V}_{22})\, e^{\xi_2^2} \operatorname{erfc} \xi_2 - (\hat{W}_2/2\hat{V}_{22})\, e^{\xi_3^2} \operatorname{erfc} \xi_3 \right\}$$

$$- \gamma\, e^{-\hat{x}/\hat{\tau}_c} \left\{ (1 + 2\,\xi_3^2)\, e^{\xi_3^2} \operatorname{erfc} \xi_3 - 2\,\xi_3/\sqrt{\pi} \right\}$$

$$+ \gamma\, 4\sqrt{\pi}\, \hat{V}_{22}\, \hat{x} \cdot F_2(\hat{x}) \Bigg] \qquad \text{(A-17)}$$

where $\xi_2 = 2\,\hat{V}_{12}\,\hat{x}$, $\xi_3 = 2\,\hat{V}_{13}\,\hat{x} = \hat{W}_2\,\hat{x} = \beta_2$,

and $F_2(\hat{x})$ is given by Eq. (A-13).

For $\hat{V}_{21} = 0$ and $\hat{V}_{22} = 0$,

$$g'_{42}(\hat{x}) = \left[Q_2/Q_1 + \gamma\,(1 - e^{-\hat{x}/\hat{\tau}_c}) \right] \cdot$$

$$e^{-\xi_2^2} \left\{ (1 + 2\,\xi_2^2)\, e^{\xi_2^2} \operatorname{erfc} \xi_2 - 2\,\xi_2/\sqrt{\pi} \right\} \qquad \text{(A-18)}$$

where $\xi_2 = \hat{W}_2\,\hat{x} = \beta_2$.

In Eqs. (A-7), (A-13), and (A-16), t is a parameterized integration variable. The integrand functions in these equations have singularities at the end-points t=0 and t=1 of the integration domain in t. Because of their complexity, these integrations cannot be carried out analytically; therefore, they should be evaluated by numerical integration to a sufficiently high degree of accuracy.

A computer-library subroutine named D01AJF, developed by the Numerical Algorithms Group (NAG), is utilized in PEM (Version 82360) for numerical integration. This general purpose integrator routine, which is capable of handling the singularities, has been selected because of its accuracy and applicability. It estimates the value of a definite integral of an externally defined function over a finite range, to a specified absolute or relative accuracy, using Gauss-Kronrod rules in an adaptive strategy with extrapolation. Further details of this subroutine can be found in Appendix D.

In the limit, when $V_{di} = W_i = 0$ and $\tau_c = \infty$, the algorithms for g'_{21}, g'_{22}, g'_{41}, and g'_{42} (defined above) reduce to the familiar Gaussian-plume diffusion algorithms currently used in EPA air quality assessment models. Thus the new algorithms given in this section may be thought of as extensions of the latter to include deposition, sedimentation, and chemical transformation.

It should be noted that the algorithms for g'_{41} and g'_{42} are also used in Eqs. (6) and (8) of Section 2.3.2 to calculate ground-level concentrations from area sources. In these equations, V_{d1} and V_{d2} should be non-zero to avoid singularities.

REFERENCE

Rao, K. S., 1982: Plume Concentration Algorithms with Deposition, Sedimentation, and Chemical Transformation. EPA-______________, U.S. Environmental Protection Agency, Research Triangle Park, NC; NOAA Tech. Memo. ERL ARL-___; ATDL Contribution File No. 82/27, 87 pp.

APPENDIX B

PLUME RISE EQUATIONS

PEM calculates plume rise from equations given by Briggs (1969, 1975). These equations are listed below. For details, the user should consult the references cited.

For unstable/neutral atmosphere, with a buoyancy-dominated plume,

$$\Delta h(x) = 1.6\ F^{1/3}\ x^{2/3}\ U^{-1}\ , \quad \text{for } x < 3.5x^* \tag{B-1}$$

and

$$\Delta h_{MAX} = 1.6\ F^{1/3}\ (3.5x^*)^{2/3}\ U^{-1}\ , \quad \text{for } x \geqq 3.5x^* \tag{B-2}$$

where

$$\begin{aligned} x^* &= 14\ F^{5/8} \qquad \text{if } F < 55\ m^4/s^3, \text{ and} \\ x^* &= 34\ F^{2/5} \qquad \text{if } F \geqq 55\ m^4/s^3. \end{aligned} \tag{B-3}$$

For stable atmosphere, with a buoyancy-dominated plume,

$$\Delta h(x) = 1.6\ F^{1/3}\ x^{2/3}\ U^{-1} \tag{B-4}$$

and

$$\Delta h_{MAX} = 2.6\ \left(\frac{F}{U\ s}\right)^{1/3} \tag{B-5}$$

where $s = 0.02\ g/T_A$ for E-stability,

(B-6)

and $s = 0.035\ g/T_A$ for F-stability.

For unstable/neutral atmosphere, with a momentum-dominated plume,

$$\Delta h(x) = 3.78\ \left[\frac{V^2}{U(V+3U)}\right]^{2/3} \left(\frac{xR^2}{2}\right)^{1/3} \qquad (B-7)$$

and

$$\Delta h_{MAX} = 6RV/U \qquad (B-8)$$

For stable atmosphere, with a momentum-dominated plume,

$$\Delta h_{MAX} = 1.5\ (VR)^{2/3}\ U^{-1/3}\ s^{-1/6} \qquad (B-9)$$

where s is defined in Eq. (B-6).

The variables used in the above equations are defined below:

$$F = gVR^2\ (T-T_A)\ /T \qquad (B-10)$$

is the plume buoyancy flux at the stack exit, m^4/s^3

g = acceleration due to gravity, 9.8 m/s^2

Δh = plume rise, m

Δh_{MAX} = maximum plume rise, m

R = inside radius of stack exit, m

T = plume temperature at stack exit, °K

T_A = ambient temperature, °K

U = mean wind speed at physical stack height, m

V = plume velocity at stack exit, m/s

x = downwind distance, m

REFERENCES

Briggs, G. A., 1969: Plume Rise. AEC Critical Review Series. Available as TID-25075 from NTIS, Springfield, VA, 81 pp.

Briggs, G. A., 1975: Plume Rise Predictions. Lectures on Air Pollution and Environmental Impact Analyses, D. A. Haugen, Workshop Coordinator, Amer. Meteorol. Soc., Boston, MA, 59-111.

APPENDIX C

SURFACE DEPOSITION FLUXES, AND DEPOSITION AND SETTLING VELOCITIES

C.1 SURFACE DEPOSITION FLUXES

The surface deposition fluxes of the primary and the secondary pollutants at ground level receptors are calculated directly as

$$D_1(\hat{x},\hat{y}) = V_{d1} \cdot C_1(\hat{x},\hat{y},0) \tag{C-1}$$

$$D_2(\hat{x},\hat{y}) = V_{d2} \cdot C_2(\hat{x},\hat{y},0) \tag{C-2}$$

D gives the amount of pollutant deposited per unit time per unit surface area, and is usually calculated as kg/km^2-hr, while seasonal estimates are expressed as kg/km^2-month. The estimation of the monthly or yearly surface deposition fluxes at a given downwind distance x from the source in a given wind-directional sector requires the knowledge of the fraction of the time that a mean wind of a given magnitude blows in that direction in a month or a year, respectively. To obtain D in kg/km^2-hr when V_d is given in cm/s and C in g/m^3, the right-hand side of the equations should be multiplied by 36000. To obtain D in μg/m^2-hr when V_d is given in cm/s and C in μg/m^3, the corresponding multiplication factor is 36. For D calculations, the ground-level receptor is generally defined as any receptor which is not higher than 1 meter above the local ground-level elevation.

PEM calculates the surface deposition fluxes of one or two pollutants. These values are printed in a map or list form, as specified by the user, in the same way the program prints the concentrations. The flux units are generally $\mu g/m^2$-hr; however, if these values are too large to be clearly printed in a map format, then the program converts them into kg/km^2-hr before printing.

C.2 DEPOSITION AND SETTLING VELOCITIES

The values of the settling and deposition velocities primarily depend on the particle diameter d. In the trivial case of $W = V_d = 0$, settling and deposition effects are negligible. For very small particles ($d < 0.1$ μm), gravitational settling can be neglected, and dry deposition occurs primarily due to nongravitational effects. In this case, $W = 0$ but $V_d > 0$. For small to medium-sized particles ($d = 0.1 \sim 50$ μm), $0 < W < V_d$; deposition is enhanced here beyond that due to gravitational settling, primarily because of increased turbulent transfer resulting from surface roughness. For larger particles ($d > 50$ μm), it is generally assumed that $V_d = W > 0$, since gravitational settling is the dominant deposition mechanism. When $W > V_d > 0$, re-entrainment of the deposited particles from the surface back into the atmosphere is implied, as in a dust storm, for example. The first four types of model parameters given above are widely used in atmospheric dispersion and deposition of particulate material. The deposition of gases is a special case of the particulate problem with W = 0. Thus, one has to carefully select the values of W and V_d for use in the models. A more complete discussion of these model parameters is given by Rao (1982).

REFERENCE

Rao, K. S., 1982: Plume Concentration Algorithms with Deposition, Sedimentation, and Chemical Transformation. EPA-____________, U.S. Environmental Protection Agency, Research Triangle Park, NC; NOAA Tech. Memo. ERL ARL-___; ATDL Contribution File No. 82/27, 87 pp.

APPENDIX D

D01AJF – NAG FORTRAN Library Routine Document

NOTE: before using this routine, please read the appropriate implementation document to check the interpretation of bold *italicised* terms and other implementation-dependent details. The routine name may be precision-dependent.

1. Purpose

D01AJF is a general-purpose integrator which calculates an approximation to the integral of a function F(x) over a finite interval (A,B):

$$I = \int_A^B F(x)\,dx.$$

2. Specification

```
      SUBROUTINE D01AJF (F, A, B, EPSABS, EPSREL, RESULT, ABSERR,
     1   W, LW, IW, LIW, IFAIL)
C     INTEGER LW, IW(LIW), LIW, IFAIL
C     real F, A, B, EPSABS, EPSREL, RESULT, ABSERR, W(LW)
C     EXTERNAL F
```

---

3. Description

D01AJF is based upon the QUADPACK [3] routine DQAGS. It is an adaptive routine, using the Gauss 10-point and Kronrod 21-point rules. The algorithm, described in [1], incorporates a global acceptance criterion (as defined by Malcolm and Simpson [2]) together with the ϵ-algorithm [4] to perform extrapolation. The local error estimation is described in [3].

The routine is suitable as a general purpose integrator, and can be used when the integrand has singularities, especially when these are of algebraic or logarithmic type.

4. References

[1] DE DONCKER, E.
An Adaptive Extrapolation Algorithm for Automatic Integration.
Signum Newsletter 13, No. 2, pp. 12-18, 1978.

[2] MALCOLM, M.A. and SIMPSON, R.B.
Local versus Global Strategies for Adaptive Quadrature.
A.C.M. Trans. Math. Software 1, pp. 129-146, 1976.

[3] PIESSENS, R., DE DONCKER, E., ÜBERHUBER, C. and KAHANER, D.
'QUADPACK', A Quadrature Subroutine Package.
To be published, 1980.

[4] WYNN, P.
On a Device for Computing the $e_m(S_n)$ Transformation.
M.T.A.C, 10, pp. 91-96, 1956.

5. Parameters

F – ***real*** FUNCTION, supplied by the user.

F must return the value of the integrand at a given point.

Its specification is:

real FUNCTION F(X)
real X

X – ***real.***

On entry, X specifies the point at which the integrand value is required by D01AJF. X must not be reset by F.

F must be declared as EXTERNAL in the (sub)program from which D01AJF is called.

A – ***real.***

On entry, A must specify the lower limit of integration.

Unchanged on exit.

B – ***real.***

On entry, B must specify the upper limit of integration.

Unchanged on exit.

EPSABS – ***real.***

On entry, EPSABS must specify the absolute accuracy required. If EPSABS is negative, the absolute value is used. See Section 10.

Unchanged on exit.

EPSREL – ***real***.

On entry, EPSREL must specify the relative accuracy required. If EPSREL is negative, the absolute value is used. See Section 10.

Unchanged on exit.

RESULT – ***real***.

On exit, RESULT contains the approximation to the integral I.

ABSERR – ***real***.

On exit, ABSERR contains an estimate of the modulus of the absolute error, which should be an upper bound for $|I-\text{RESULT}|$.

W – ***real*** array of DIMENSION (LW).

Used as workspace.

LW – INTEGER.

On entry, LW must specify the dimension of W as declared in the calling (sub)program. LW/4 is an upper bound for the number of subintervals into which the interval of integration is divided. A value in the range 800 to 2000 is adequate for most problems. The more difficult the integrand, the larger LW should be. Trivially $\text{LW} \geq 4$. See IW below.

LW is unchanged on exit.

IW – INTEGER array of DIMENSION (LIW).

Used as workspace.

On exit, IW(1) contains the amount of ***real*** workspace actually used (the smallest possible value of LW).

LIW – INTEGER.

On entry, LIW must specify the dimension of IW, as declared in the calling (sub)program. $\text{LIW} \geq \text{LW}/8 + 2$.

Unchanged on exit.

IFAIL – INTEGER.

Before entry, IFAIL must be assigned a value. For users not familiar with this parameter (described in Chapter P01) the recommended value is 0.

Unless the routine detects an error (see next section), IFAIL contains 0 on exit.

6. Error Indicators and Warnings

Errors detected by the routine:–

IFAIL = 1

The maximum number of subdivisions allowed with the given workspace has been reached without the accuracy requirements being achieved. Look at the integrand in order to determine the integration difficulties. If the position of a local difficulty within the interval can be determined (e.g. a singularity of the integrand or its derivative, a peak, a discontinuity...) one will probably gain from splitting up the interval at this point and calling the integrator on the subranges. If necessary, another integrator which is designed for handling the type of difficulty involved, must be used. Alternatively consider relaxing the accuracy requirements specified by EPSABS and EPSREL, or increasing the amount of workspace.

IFAIL = 2

Roundoff error prevents the requested tolerance from being achieved. The error may be under-estimated. Consider requesting less accuracy.

IFAIL = 3

Extremely bad local integrand behaviour causes a very strong subdivision around one (or more) points of the interval. The same advice applies as in the case of IFAIL = 1.

IFAIL = 4

The requested tolerance cannot be achieved, because the extrapolation does not increase the accuracy satisfactorily; the returned result is the best which can be obtained. The same advice applies as in the case of IFAIL = 1.

IFAIL = 5

The integral is probably divergent, or slowly convergent. It must be noted that divergence can also occur with any non-zero value of IFAIL.

IFAIL = 6

On entry, $\text{LW} < 4$, or $\text{LIW} < \text{LW}/8 + 2$.

7. Auxiliary Routines

This routine calls NAG Library routines D01AJV, D01AJX, D01AJY, D01AJZ, P01AAF, X02AAF, X02ABF and X02ACF.

8. Timing

This depends on the integrand and the accuracy required.

9. Storage

The storage required by internally declared arrays is 107 *real* elements.

10. Accuracy

The routine cannot guarantee, but in practice usually achieves, the following accuracy:

$|I-\text{RESULT}|\leq tol$

where

$$tol = \max(|\text{EPSABS}|, |\text{EPSREL}| \times |I|)$$

and EPSABS and EPSREL are user-specified absolute and relative error tolerance. Moreover it returns the quantity ABSERR which, in normal circumstances, satisfies $|I-\text{RESULT}| \leq \text{ABSERR} \leq tol$.

11. Further Comments

Labelled COMMON block AD01AJ is used by this routine and must therefore be avoided by the user.

12. Keywords

Quadrature, Extrapolation, Globally Adaptive, Singularities.

---

13. Example

To compute $\displaystyle\int_0^{2\pi} \frac{x.sin(30x)}{\sqrt{(1-(\frac{x}{2\pi})^2)}}\,dx$

WARNING: This **single precision** example program may require amendment for certain implementations. The results produced may not be the same. If in doubt, please seek further advice (see **Essential Introduction** to the Library Manual).

13.1. Program Text

```
C     D01AJF EXAMPLE PROGRAM TEXT
C     MARK 8 RELEASE. NAG COPYRIGHT 1979.
C     .. SCALARS IN COMMON ..
      REAL PI
      INTEGER KOUNT
C     ..
C     .. LOCAL SCALARS ..
      REAL A, ABSERR, B, EPSABS, EPSREL, EX, EXACT, RESULT
      INTEGER IFAIL, NOUT
C     .. LOCAL ARRAYS ..
      REAL W(800)
      INTEGER IW(102)
C     .. FUNCTION REFERENCES ..
      REAL X01AAF
C     .. SUBROUTINE REFERENCES ..
C     D01AJF
C     ..
      EXTERNAL FST
      COMMON /TELNUM/ PI, KOUNT
      DATA EXACT /-0.2543259618893530E+01/
      DATA NOUT /6/
      WRITE (NOUT,99999)
      PI = X01AAF(PI)
      EPSABS = 0.E0
      EPSREL = 1.E-04
      A = 0.E0
      B = 2.E0*PI
      KOUNT = 0
      IFAIL = 1
      CALL D01AJF(FST, A, B, EPSABS, EPSREL, RESULT, ABSERR, W,
     * 800, IW, 102, IFAIL)
      WRITE (NOUT,99998) A, B, EPSABS, EPSREL
      WRITE (NOUT,99997) RESULT, ABSERR, KOUNT, IW(1), IFAIL
      EX = ABS(EXACT-RESULT)
      WRITE (NOUT,99996) EX
      STOP
99999 FORMAT (4(1X/), 31H D01AJF EXAMPLE PROGRAM RESULTS/1X)
99998 FORMAT (1H , 2X, 1HA, 6X, 31H- LOWER LIMIT OF INTEGRATION = ,
     * F10.4/1H , 2X, 1HB, 6X, 31H- UPPER LIMIT OF INTEGRATION = ,
     * F10.4/1H , 2X, 39HEPSABS - ABSOLUTE ACCURACY REQUESTED = ,
     * E9.2/1H , 2X, 39HEPSREL - RELATIVE ACCURACY REQUESTED = ,
     * E9.2/)
99997 FORMAT (1H , 2X, 41HRESULT - APPROXIMATION TO THE INTEGRAL = ,
     * E14.5/1H , 2X, 42HABSERR - ESTIMATE OF THE ABSOLUTE ERROR = ,
     * E10.3/1H , 2X, 42HKOUNT  - NUMBER OF FUNCTION EVALUATIONS = ,
     * I4/1H , 2X, 43HIW(1)  - ELEMENTS OF REAL WORKSPACE USED = ,
     * I4/1H , 2X, 22HIFAIL  - ERROR FLAG = , I4/)
99996 FORMAT (1H , 7X, 27H  - EXACT ABSOLUTE ERROR = , E10.3)
      END
      REAL FUNCTION FST(X)
C     .. SCALAR ARGUMENTS ..
      REAL X
C     ..
C     .. SCALARS IN COMMON ..
      REAL PI
      INTEGER KOUNT
C     ..
C     .. FUNCTION REFERENCES ..
      REAL SIN, SQRT
C     ..
      COMMON /TELNUM/ PI, KOUNT
      KOUNT = KOUNT + 1
      FST = X*SIN(30.E0*X)/SQRT(1.E0-X**2/(4.E0*PI**2))
      RETURN
      END
C      D01AJF EXAMPLE PROGRAM TEXT
C      MARK 8 RELEASE. NAG COPYRIGHT 1979.
```

13.2. Program Data

None.

13.3. Program Results

```
 D01AJF EXAMPLE PROGRAM RESULTS

  A       - LOWER LIMIT OF INTEGRATION =      0.0000
  B       - UPPER LIMIT OF INTEGRATION =     6.2832
  EPSABS - ABSOLUTE ACCURACY REQUESTED =  0.00E 00
  EPSREL - RELATIVE ACCURACY REQUESTED =  0.10E-03

  RESULT - APPROXIMATION TO THE INTEGRAL =   -0.25433E 01
  ABSERR - ESTIMATE OF THE ABSOLUTE ERROR =  0.128E-04
  KOUNT  - NUMBER OF FUNCTION EVALUATIONS =  777
  IW(1)  - ELEMENTS OF REAL WORKSPACE USED =   76
  IFAIL  - ERROR FLAG =     0

        - EXACT ABSOLUTE ERROR =  0.893E-08
```

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APPENDIX E

INPUT AND OUTPUT LISTINGS OF EXAMPLE PROBLEMS

TABLE 11

INPUT DATA FOR EXAMPLE PROBLEM 1

CARD IMAGES

```
CONTROL CARDS
  1  TITLE        PEM EXAMPLE 1   CHEMICAL TRANSFORMATION GAS TO SMALL PARTICLE
  2  OPTIONS          1    1    1    1    0    2    0    0    1    0    1    1    1
  3  GRID                 0.        0.        25        25       .04        0.        0.
  4  POLLUTANTS       2    1       1.0       0.0       0.1       0.0       1.0       1.5
  5  SCALING             1.0       1.0        0.        0.        0.        0.
  6  LABELS       GAS 1                                  GAS 2

SCENARIO CARDS
                      4    3    9                         15          1.    1000.

AREA SOURCE CARDS
                         .38       .02      120.       0.5      0.05
                  BLANK CARD TO SIGNAL END OF AREA SOURCE INVENTORY

POINT SOURCE CARDS
                        .20      0.0      1.0     0.10     15.0      1.0      5.0     32.4 STACK 1
                        .66      .04      1.0     0.10     10.0      3.0      0.5     32.4 STACK 2
                  BLANK CARD TO SIGNAL END OF POINT SOURCE INVENTORY
```

TABLE 12

OUTPUT LISTING FOR EXAMPLE PROBLEM 1

```
                  PEM   (VERSION  82360)


                POLLUTION EPISODIC MODEL


                        INCLUDING
  DEPOSITION, SEDIMENTATION, AND CHEMICAL TRANSFORMATION
                      OF POLLUTANTS
```

```
                                   POLLUTION EPISODIC MODEL

INPUT CONTROL PARAMETERS:  PEM EXAMPLE 1   CHEMICAL TRANSFORMATION GAS TO SMALL PARTICLE

    AVERAGING TIME OPTION: NTOPT=1

          A SCENARIO IS A SET OF METEOROLOGICAL DATA FOR ONE HOUR

      1  1 HOUR: CONCENTRATIONS ARE CALCULATED FOR EACH SCENARIO
      2  24 HOURS: CONCENTRATIONS CALCULATED FOR 24 SCENARIOS ARE AVERAGED
      3  VARIABLE: CONCENTRATIONS CALCULATED FOR A GIVEN NUMBER (2 TO 24) OF SCENARIOS ARE AVERAGED

    WIND DIRECTION OPTION: NWDOPT=1

      0  DIRECTION IN DEGREES TO BE SPECIFIED FOR EACH SCENARIO
      1  SECTOR NUMBER TO BE SPECIFIED FOR EACH SCENARIO
     2-7 DIRECTION IN DEGREES TO BE SPECIFIED FOR THE FIRST OF FOUR SUB-SCENARIOS.
          FOR EACH SUCCEEDING SUB-SCENARIO, WIND DIRECTION IS AUTOMATICALLY INCREASED
          BY 90,45,30,15,10,OR 5 DEGREES, DEPENDING ON THE OPTION NUMBER SELECTED.

    WIND SPEED OPTION: NWSOPT=1

      0  SPEED IN M/S TO BE SPECIFIED FOR EACH SCENARIO
      1  WIND SPEED CLASS NUMBER TO BE SPECIFIED FOR EACH SCENARIO

    NUMBER OF SCENARIOS: NSCEN= 1

    STACK-TIP DOWNWASH ALGORITHM OPTION: NSTDWN=0

      0  ALGORITHM IS IN EFFECT
      1  ALGORITHM IS NOT USED

    RECEPTOR GRID:         COLUMNS: LX= 25    ROWS: LY= 25
                           SPACING: GRID=  0.040 KM
                           SOUTHWEST CORNER    XRSWC=    0.0   KM W
                                               YRSWC=    0.0   KM S

    POTENTIAL TEMPERATURE GRADIENT: DTDZ(1)=   0.020 DEG/M    STABILITY CLASS E
                                    DTDZ(2)=   0.035 DEG/M    STABILITY CLASS F
```

```
                                 POLLUTION EPISODIC MODEL

INPUT CONTROL PARAMETERS:  PEM EXAMPLE 1   CHEMICAL TRANSFORMATION GAS TO SMALL PARTICLE

     NUMBER OF POLLUTANTS: NPOL=2
                                         POLLUTANT-1: GAS 1                    POLLUTANT-2: GAS 2

     AREA SOURCE SCALING FACTOR:            ASCALE=    1.000                      ASCALE=    1.000
     CALIBRATION COEFFICIENTS:           A=     0.0     B=      0.0         A=     0.0     B=      0.0
     CALIBRATION IDENTIFICATION:
     DEPOSITION VELOCITY (CM/S):              VD1=   1.000                      VD2=   0.100
     SETTLING VELOCITY (CM/S):                 W1=   0.0                         W2=   0.0

     CHEMICAL TRANSFORMATION OPTION: ICT=1

        NPOL=2
          ICT=0  CHEMICAL TRANSFORMATION LOSS OF POLLUTANTS IS IGNORED
          ICT=1  FIRST-ORDER CHEMICAL TRANSFORMATION OF POLLUTANT-1 TO POLLUTANT-2 IS CONSIDERED

     CHEMICAL TRANSFORMATION RATE: XKT=  1.000 PERCENT/HR

     RATIO OF MOLECULAR WEIGHTS OF POLLUTANT-2 (PRODUCT) TO POLLUTANT-1 (REACTANT): GAMMA= 1.500


    OUTPUT OPTIONS SELECTED:

       NARRAY=2  MAPS OF CONCENTRATION AND SURFACE DEPOSITION FLUX AT EACH RECEPTOR IN THE GRID,
                 UNCALIBRATED ONLY
       NPRINT=1  LIST OF POINT SOURCE PARAMETERS AND EFFECTIVE STACK HEIGHTS
                 PRINTED AT BEGINNING OF EACH SCENARIO
       NMAX=1    LIST OF RECEPTORS WITH HIGHEST CONCENTRATION AND SURFACE DEPOSITION FLUX
                 FOR EACH SCENARIO - PRINTED AT END OF RUN
```

```
                                     POLLUTION EPISODIC MODEL

INPUT SCENARIO PARAMETERS:  PEM EXAMPLE 1   CHEMICAL TRANSFORMATION GAS TO SMALL PARTICLE

                    WIND DIRECTIONS                              WIND SPEED CLASSES                STABILITY CLASSES

     SECTOR    DIRECTION        SECTOR     DIRECTION          CLASS   SPEED    CLASS                CLASS
     NUMBER        (DEG)        NUMBER         (DEG)          INDEX   (M/S)   INTERVAL(KT)          INDEX   CLASS

       1    N        0.0           9    S      180.0
       2    NNE     22.5          10    SSW    202.5            1      1.50       0-3                 1      A
       3    NE      45.0          11    SW     225.0            2      2.46       4-6                 2      B
       4    ENE     67.5          12    WSW    247.5            3      4.47       7-10                3      C
       5    E       90.0          13    W      270.0            4      6.93      11-16                4      DD (DAY)
       6    ESE    112.5          14    WNW    292.5            5      9.61      17-21                5      DN (NIGHT)
       7    SE     135.0          15    NW     315.0            6     12.52     OVER 21               6      E
       8    SSE    157.5          16    NNW    337.5                                                 7      F


 SCENARIO   STABILITY   WIND SPEED     WIND       WIND       WIND        AMBIENT         INVERSION          MIXING
  NUMBER      CLASS       CLASS        SPEED     SECTOR    DIRECTION    TEMPERATURE  PENETRATION FACTOR    HEIGHT
                                       (M/S)                 (DEG)        (DEG C)                            (M)

    1          DD           3          4.470       9        180.00        15.00           1.000           1000.0
```

```
                                       POLLUTION EPISODIC MODEL

INPUT AREA SOURCE PARAMETERS:  PEM EXAMPLE 1   CHEMICAL TRANSFORMATION GAS TO SMALL PARTICLE

                                                                POLLUTANT-1                   POLLUTANT-2
AREA SOURCE       COORDINATES         LENGTH OF SIDE           EMISSION RATE                 EMISSION RATE
  NUMBER        X(KM)     Y(KM)            (M)             INPUT (G/S)     SCALED        INPUT (G/S)     SCALED

    1            0.38      0.02           120.00              0.500         0.500           0.050         0.050

 SUMS OF THE AREA SOURCE EMISSION RATES IN THIS RUN           0.500         0.500           0.050         0.050
```

```
                                POLLUTION EPISODIC MODEL

INPUT POINT SOURCE PARAMETERS:  PEM EXAMPLE 1   CHEMICAL TRANSFORMATION GAS TO SMALL PARTICLE

 POINT SOURCE          COORDINATES          EMISSION RATE       EMISSION RATE     HEIGHT    DIAMETER     EXIT VEL      EXIT TEMP
NUMBER   LABEL        X(KM)     Y(KM)     POLLUTANT-1 (G/S)  POLLUTANT-2 (G/S)    (M)        (M)         (M/S)        (DEG C)

   1     STACK 1      0.20      0.0             1.000              0.100          15.00      1.000        5.000         32.400
   2     STACK 2      0.68      0.04            1.000              0.100          10.00      3.000        0.500         32.400

 SUMS OF THE POINT SOURCE EMISSION RATES        2.000 G/S          0.200 G/S
```

```
                                        POLLUTION EPISODIC MODEL

    OUTPUT:  PEM EXAMPLE 1   CHEMICAL TRANSFORMATION GAS TO SMALL PARTICLE

    SCENARIO 1    POINT SOURCE PLUME RISE CALCULATIONS
                      MIXING HEIGHT: HMIX=1000.00 M
                      IF MAXIMUM EFFECTIVE SOURCE HEIGHT IS GREATER THAN  1000.0 M, THE SOURCE IS IGNORED

             SOURCE          EMISSION RATES                                                                        WIND SPEED AT     MAXIMUM
POINT      COORDINATES       POL-1       PCL-2       HEIGHT   DIAMETER   EXIT VEL   EXIT TEMP       DOMINANT       STACK HEIGHT     EFFECTIVE
SOURCE   X(KM)    Y(KM)      (G/S)       (G/S)        (M)       (M)       (M/S)     (DEG K)        INFLUENCE          (M/S)       SOURCE HEIGHT(M)

  1      0.20     0.0         1.00        0.10       15.00     1.000      5.000     305.55   BUOYANCY DOWNWASH      4.947            17.33
  2      0.68     0.04        1.00        0.10       10.00     3.000      0.500     305.55   BUOYANCY DOWNWASH      4.470            10.00
```

```
PEM OUTPUT:  SECTION 1 OF 1, SCENARIO  1  PEM EXAMPLE 1   CHEMICAL TRANSFORMATION GAS TO SMALL PARTICLE
STABILITY=DD, WIND SPD= 4.47 M/S, WIND DIR=180.00 DEG, MIXING HT= 1000.0 M, AVERAGING TIME=  1 HR.      POLLUTANT-1: GAS 1
UNCALIBRATED CONCENTRATION - MICROGRAMS PER CUBIC METER
              0.0     0.08    0.16    0.24    0.32    0.40    0.48    0.56    0.64    0.72    0.80    0.88    0.96

     0.96      0   1   5  12  21  25  21  12   5   1   0   0   0   1   5  15  27  33  27  15   5   1   0   0   0       0.96
     0.92      0   1   4  12  22  27  22  12   4   1   0   0   0   1   5  15  28  35  28  15   5   1   0   0   0       0.92
     0.88      0   1   4  12  23  29  23  12   4   1   0   0   0   1   5  15  30  38  30  15   5   1   0   0   0       0.88
     0.84      0   1   4  12  24  31  24  12   4   1   0   0   0   1   4  15  31  41  31  15   4   1   0   0   0       0.84
     0.80      0   1   3  12  25  33  25  12   3   1   0   0   0   0   3  14  33  44  33  14   3   0   0   0   0       0.80
     0.76      0   0   3  11  26  35  26  11   3   0   0   0   0   0   3  14  35  48  35  14   3   0   0   0   0       0.76
     0.72      0   0   2  11  27  37  27  11   2   0   0   0   0   0   2  13  37  52  37  13   2   0   0   0   0       0.72
     0.68      0   0   2  10  28  40  28  10   2   0   0   0   0   0   2  12  39  57  39  12   2   0   0   0   0       0.68
     0.64      0   0   1   9  29  43  29   9   1   0   0   0   0   0   1  11  41  63  41  11   1   0   0   0   0       0.64
     0.60      0   0   1   8  30  47  30   8   1   0   0   0   0   0   1  10  43  70  43  10   1   0   0   0   0       0.60
     0.56      0   0   1   7  31  51  31   7   1   0   0   0   0   0   0   8  44  78  44   8   0   0   0   0   0       0.56
     0.52      0   0   0   6  31  55  31   6   0   0   0   0   0   0   0   6  46  89  46   6   0   0   0   0   0       0.52
     0.48      0   0   0   4  31  60  31   4   0   0   0   0   0   0   0   5  47 101  47   5   0   0   0   0   0       0.48
     0.44      0   0   0   3  30  65  30   3   0   0   0   0   0   0   0   3  46 117  46   3   0   0   0   0   0       0.44
     0.40      0   0   0   2  28  70  28   2   0   0   0   0   0   0   0   2  44 135  44   2   0   0   0   0   0       0.40
     0.36      0   0   0   1  25  75  25   1   0   0   0   0   0   0   0   0  40 158  40   0   0   0   0   0   0       0.36
     0.32      0   0   0   0  20  78  20   0   0   0   0   0   0   0   0   0  32 186  32   0   0   0   0   0   0       0.32
     0.28      0   0   0   0  13  78  13   0   0   0   9   9   9   0   0   0  21 218  21   0   0   0   0   0   0       0.28
     0.24      0   0   0   0   7  71   7   0   0   0  21  21  21   0   0   0  10 250   9   0   0   0   0   0   0       0.24
     0.20      0   0   0   0   2  56   2   0   0   0  38  38  38   0   0   0   0 269   0   0   0   0   0   0   0       0.20
     0.16      0   0   0   0   0  30   0   0   0   0  62  62  62   0   0   0   0 230   0   0   0   0   0   0   0       0.16
     0.12      0   0   0   0   0   7   0   0   0   0 252 252 252   0   0   0   0  83   0   0   0   0   0   0   0       0.12
     0.08      0   0   0   0   0   0   0   0   0   0 234 234 234   0   0   0   0   0   0   0   0   0   0   0   0       0.08
     0.04      0   0   0   0   0   0   0   0   0   0 201 201 201   0   0   0   0   0   0   0   0   0   0   0   0       0.04
     0.0       0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0       0.0
              0.0     0.08    0.16    0.24    0.32    0.40    0.48    0.56    0.64    0.72    0.80    0.88    0.96
```

```
PEM OUTPUT:  SECTION 1 OF 1, SCENARIO  1  PEM EXAMPLE 1   CHEMICAL TRANSFORMATION GAS TO SMALL PARTICLE
STABILITY=DC, WIND SPD= 4.47 M/S, WIND DIR=180.00 DEG, MIXING HT= 1000.0 M, AVERAGING TIME=  1 HR.      POLLUTANT-1: GAS 1
UNCALIBRATED SURFACE DEPOSITION FLUX - KILOGRAMS PER SQUARE KILOMETER PER HOUR

             0.0     0.08    0.16    0.24    0.32    0.40    0.48    0.56    0.64    0.72    0.80    0.88    0.96

   0.96        0   0   0   0   1   1   1   0   0   0   0   0   0   0   0   1   1   1   1   1   0   0   0   0   0        0.96
   0.92        0   0   0   0   1   1   1   0   0   0   0   0   0   0   0   1   1   1   1   1   0   0   0   0   0        0.92
   0.88        0   0   0   0   1   1   1   0   0   0   0   0   0   0   0   1   1   1   1   1   0   0   0   0   0        0.88
   0.84        0   0   0   0   1   1   1   0   0   0   0   0   0   0   0   1   1   1   1   1   0   0   0   0   0        0.84
   0.80        0   0   0   0   1   1   1   0   0   0   0   0   0   0   0   1   1   2   1   1   0   0   0   0   0        0.80
   0.76        0   0   0   0   1   1   1   0   0   0   0   0   0   0   0   0   1   2   1   0   0   0   0   0   0        0.76
   0.72        0   0   0   0   1   1   1   0   0   0   0   0   0   0   0   0   1   2   1   0   0   0   0   0   0        0.72
   0.68        0   0   0   0   1   1   1   0   0   0   0   0   0   0   0   0   1   2   1   0   0   0   0   0   0        0.68
   0.64        0   0   0   0   1   2   1   0   0   0   0   0   0   0   0   0   1   2   1   0   0   0   0   0   0        0.64
   0.60        0   0   0   0   1   2   1   0   0   0   0   0   0   0   0   0   2   3   2   0   0   0   0   0   0        0.60
   0.56        0   0   0   0   1   2   1   0   0   0   0   0   0   0   0   0   2   3   2   0   0   0   0   0   0        0.56
   0.52        0   0   0   0   1   2   1   0   0   0   0   0   0   0   0   0   2   3   2   0   0   0   0   0   0        0.52
   0.48        0   0   0   0   1   2   1   0   0   0   0   0   0   0   0   0   2   4   2   0   0   0   0   0   0        0.48
   0.44        0   0   0   0   1   2   1   0   0   0   0   0   0   0   0   0   2   4   2   0   0   0   0   0   0        0.44
   0.40        0   0   0   0   1   3   1   0   0   0   0   0   0   0   0   0   2   5   2   0   0   0   0   0   0        0.40
   0.36        0   0   0   0   1   3   1   0   0   0   0   0   0   0   0   0   1   6   1   0   0   0   0   0   0        0.36
   0.32        0   0   0   0   1   3   1   0   0   0   0   0   0   0   0   0   1   7   1   0   0   0   0   0   0        0.32
   0.28        0   0   0   0   0   3   0   0   0   0   0   0   0   0   0   0   1   8   1   0   0   0   0   0   0        0.28
   0.24        0   0   0   0   0   3   0   0   0   0   1   1   1   0   0   0   0   9   0   0   0   0   0   0   0        0.24
   0.20        0   0   0   0   0   2   0   0   0   0   1   1   1   0   0   0   0  10   0   0   0   0   0   0   0        0.20
   0.16        0   0   0   0   0   1   0   0   0   0   2   2   2   0   0   0   0   8   0   0   0   0   0   0   0        0.16
   0.12        0   0   0   0   0   0   0   0   0   0   9   9   9   0   0   0   0   3   0   0   0   0   0   0   0        0.12
   0.08        0   0   0   0   0   0   0   0   0   0   8   8   8   0   0   0   0   0   0   0   0   0   0   0   0        0.08
   0.04        0   0   0   0   0   0   0   0   0   0   7   7   7   0   0   0   0   0   0   0   0   0   0   0   0        0.04
   0.0         0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0        0.0

             0.0     0.08    0.16    0.24    0.32    0.40    0.48    0.56    0.64    0.72    0.80    0.88    0.96
```

```
PEM OUTPUT:  SECTION 1 OF 1, SCENARIO  1  PEM EXAMPLE 1   CHEMICAL TRANSFORMATION GAS TO SMALL PARTICLE
STABILITY=DC, WIND SPD= 4.47 M/S, WIND DIR=180.00 DEG, MIXING HT= 1000.0 M, AVERAGING TIME=  1 HR.      POLLUTANT-2: GAS 2
UNCALIBRATED CONCENTRATION - MICROGRAMS PER CUBIC METER

              0.0     0.08    0.16    0.24    0.32    0.40    0.48    0.56    0.64    0.72    0.80    0.88    0.96
   0.96       0   0   1   1   2   3   2   1   1   0   0   0   0   0   1   2   3   4   3   2   1   0   0   0   0        0.96
   0.92       0   0   0   1   2   3   2   1   0   0   0   0   0   0   1   2   3   4   3   2   1   0   0   0   0        0.92
   0.88       0   0   0   1   3   3   3   1   0   0   0   0   0   0   1   2   3   4   3   2   1   0   0   0   0        0.88
   0.84       0   0   0   1   3   3   3   1   0   0   0   0   0   0   0   2   4   5   4   2   0   0   0   0   0        0.84
   0.80       0   0   0   1   3   4   3   1   0   0   0   0   0   0   0   2   4   5   4   2   0   0   0   0   0        0.80
   0.76       0   0   0   1   3   4   3   1   0   0   0   0   0   0   0   2   4   5   4   2   0   0   0   0   0        0.76
   0.72       0   0   0   1   3   4   3   1   0   0   0   0   0   0   0   1   4   6   4   1   0   0   0   0   0        0.72
   0.68       0   0   0   1   3   4   3   1   0   0   0   0   0   0   0   1   4   6   4   1   0   0   0   0   0        0.68
   0.64       0   0   0   1   3   5   3   1   0   0   0   0   0   0   0   1   5   7   5   1   0   0   0   0   0        0.64
   0.60       0   0   0   1   3   5   3   1   0   0   0   0   0   0   0   1   5   8   5   1   0   0   0   0   0        0.60
   0.56       0   0   0   1   3   5   3   1   0   0   0   0   0   0   0   1   5   9   5   1   0   0   0   0   0        0.56
   0.52       0   0   0   1   3   6   3   1   0   0   0   0   0   0   0   1   5  10   5   1   0   0   0   0   0        0.52
   0.48       0   0   0   0   3   6   3   0   0   0   0   0   0   0   0   1   5  11   5   1   0   0   0   0   0        0.48
   0.44       0   0   0   0   3   7   3   0   0   0   0   0   0   0   0   0   5  13   5   0   0   0   0   0   0        0.44
   0.40       0   0   0   0   3   7   3   0   0   0   0   0   0   0   0   0   5  15   5   0   0   0   0   0   0        0.40
   0.36       0   0   0   0   3   8   3   0   0   0   0   0   0   0   0   0   4  17   4   0   0   0   0   0   0        0.36
   0.32       0   0   0   0   2   8   2   0   0   0   0   0   0   0   0   0   3  20   3   0   0   0   0   0   0        0.32
   0.28       0   0   0   0   1   8   1   0   0   0   1   1   1   0   0   0   2  23   2   0   0   0   0   0   0        0.28
   0.24       0   0   0   0   1   7   1   0   0   0   2   2   2   0   0   0   1  27   1   0   0   0   0   0   0        0.24
   0.20       0   0   0   0   0   6   0   0   0   0   4   4   4   0   0   0   0  28   0   0   0   0   0   0   0        0.20
   0.16       0   0   0   0   0   3   0   0   0   0   6   6   6   0   0   0   0  24   0   0   0   0   0   0   0        0.16
   0.12       0   0   0   0   0   1   0   0   0   0  25  25  25   0   0   0   0   9   0   0   0   0   0   0   0        0.12
   0.08       0   0   0   0   0   0   0   0   0   0  24  24  24   0   0   0   0   0   0   0   0   0   0   0   0        0.08
   0.04       0   0   0   0   0   0   0   0   0   0  20  20  20   0   0   0   0   0   0   0   0   0   0   0   0        0.04
   0.0        0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0        0.0
              0.0     0.08    0.16    0.24    0.32    0.40    0.48    0.56    0.64    0.72    0.80    0.88    0.96
```

```
PEM OUTPUT:  SECTION 1 OF 1, SCENARIO  1  PEM EXAMPLE 1   CHEMICAL TRANSFORMATION GAS TO SMALL PARTICLE
STABILITY=CC, WIND SPD= 4.47 M/S, WIND DIR=180.00 DEG, MIXING HT= 1000.0 M, AVERAGING TIME=  1 HR.
UNCALIBRATED SURFACE DEPOSITION FLUX - MICROGRAMS PER SQUARE METER PER HOUR                         POLLUTANT-2: GAS 2
             0.0     0.08    0.16    0.24    0.32    0.40    0.48    0.56    0.64    0.72    0.80    0.88    0.96
   0.96      0   1   2   5   8  10   8   5   2   1   0   0   0   1   2   6  11  13  11   6   2   1   0   0   0      0.96
   0.92      0   0   2   5   9  11   9   5   2   0   0   0   0   0   2   6  12  14  12   6   2   0   0   0   0      0.92
   0.88      0   0   2   5   9  11   9   5   2   0   0   0   0   0   2   6  12  15  12   6   2   0   0   0   0      0.88
   0.84      0   0   1   5  10  12  10   5   1   0   0   0   0   0   2   6  13  17  13   6   2   0   0   0   0      0.84
   0.80      0   0   1   5  10  13  10   5   1   0   0   0   0   0   1   6  13  18  13   6   1   0   0   0   0      0.80
   0.76      0   0   1   4  10  14  10   4   1   0   0   0   0   0   1   6  14  19  14   6   1   0   0   0   0      0.76
   0.72      0   0   1   4  11  15  11   4   1   0   0   0   0   0   1   5  15  21  15   5   1   0   0   0   0      0.72
   0.68      0   0   1   4  11  16  11   4   1   0   0   0   0   0   1   5  16  23  16   5   1   0   0   0   0      0.68
   0.64      0   0   1   4  12  17  12   4   1   0   0   0   0   0   0   4  16  25  16   4   0   0   0   0   0      0.64
   0.60      0   0   0   3  12  18  12   3   0   0   0   0   0   0   0   4  17  28  17   4   0   0   0   0   0      0.60
   0.56      0   0   0   3  12  20  12   3   0   0   0   0   0   0   0   3  18  31  18   3   0   0   0   0   0      0.56
   0.52      0   0   0   2  12  21  12   2   0   0   0   0   0   0   0   3  18  35  18   3   0   0   0   0   0      0.52
   0.48      0   0   0   2  12  23  12   2   0   0   0   0   0   0   0   2  18  40  18   2   0   0   0   0   0      0.48
   0.44      0   0   0   1  12  25  12   1   0   0   0   0   0   0   0   1  18  46  18   1   0   0   0   0   0      0.44
   0.40      0   0   0   1  11  27  11   1   0   0   0   0   0   0   0   1  17  53  17   1   0   0   0   0   0      0.40
   0.36      0   0   0   0   9  29   9   0   0   0   0   0   0   0   0   0  15  61  15   0   0   0   0   0   0      0.36
   0.32      0   0   0   0   7  30   7   0   0   0   0   0   0   0   0   0  12  72  12   0   0   0   0   0   0      0.32
   0.28      0   0   0   0   5  29   5   0   0   0   4   4   4   0   0   0   8  84   8   0   0   0   0   0   0      0.28
   0.24      0   0   0   0   3  27   3   0   0   0   9   9   9   0   0   0   4  96   4   0   0   0   0   0   0      0.24
   0.20      0   0   0   0   1  21   1   0   0   0  15  15  15   0   0   0   0 102   0   0   0   0   0   0   0      0.20
   0.16      0   0   0   0   0  11   0   0   0   0  23  23  23   0   0   0   0  86   0   0   0   0   0   0   0      0.16
   0.12      0   0   0   0   0   2   0   0   0   0  91  91  91   0   0   0   0  31   0   0   0   0   0   0   0      0.12
   0.08      0   0   0   0   0   0   0   0   0   0  85  85  85   0   0   0   0   0   0   0   0   0   0   0   0      0.08
   0.04      0   0   0   0   0   0   0   0   0   0  73  73  73   0   0   0   0   0   0   0   0   0   0   0   0      0.04
   0.0       0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0      0.0
             0.0     0.08    0.16    0.24    0.32    0.40    0.48    0.56    0.64    0.72    0.80    0.88    0.96
```

```
                                    POLLUTION EPISODIC MODEL

       OUTPUT:  PEM EXAMPLE 1   CHEMICAL TRANSFORMATION GAS TO SMALL PARTICLE

       HIGHEST PREDICTED CONCENTRATION OF EACH POLLUTANT FOR EACH SCENARIO

       UNCALIBRATED CONCENTRATION IN MICROGRAMS PER CUBIC METER  -  CALIBRATION, POLLUTANT-1:
                                                                    CALIBRATION, POLLUTANT-2:

                              POLLUTANT-1: GAS 1                                          POLLUTANT-2: GAS 2
SCENARIO  WIND DIRECTION     COORDINATES            CONCENTRATION                 COORDINATES             CONCENTRATION
 NUMBER    SUB-SCENARIO    X(KM)     Y(KM)     UNCALIBRATED    CALIBRATED       X(KM)     Y(KM)      UNCALIBRATED    CALIBRATED

   1            1           0.68      0.20       268.5979         0.0            0.68      0.20         28.2320          0.0
```

```
                                  POLLUTION EPISODIC MODEL

      OUTPUT:  PEM EXAMPLE 1   CHEMICAL TRANSFORMATION GAS TO SMALL PARTICLE

      HIGHEST PREDICTED SURFACE DEPOSITION FLUX OF EACH POLLUTANT FOR EACH SCENARIO

      UNCALIBRATED VALUES IN MICROGRAMS PER SQUARE METER PER HOUR  -  CALIBRATION, POLLUTANT-1:
                                                                     CALIBRATION, POLLUTANT-2:

                                        POLLUTANT-1: GAS 1                                         POLLUTANT-2: GAS 2
    SCENARIO  WIND DIRECTION      COORDINATES          SURFACE DEPOSITION FLUX             COORDINATES          SURFACE DEPOSITION FLUX
     NUMBER    SUB-SCENARIO     X(KM)     Y(KM)      UNCALIBRATED     CALIBRATED         X(KM)     Y(KM)      UNCALIBRATED     CALIBRATED

       1            1            0.68      0.20        9669.5234         0.0              0.68      0.20        101.6351          0.0
    IHC002I STOP      0
```

TABLE 13

INPUT DATA FOR EXAMPLE PROBLEM 2

CARD IMAGES

```
CONTROL CARDS
  1  TITLE          PEM EXAMPLE 2  CHEMICAL TRANSFURMATICN GAS TC PARTICLE  3-HR AVG CONCENTRATIONS
  2  OPTICNS            3    1    1    3    0    2    0    C    1    0    0    0    1
  3  GRID                     C.        0.        25        25       2.0        0.        0.
  4  POLLUTANTS         2    1       2.C       0.0       0.5       .25      20.0       1.5
  5  SCALING                1.0       1.C        0.        0.        C.        0.
  6  LABELS         GAS                                     PARTICLE

SCENARIC CARCS
                        5    4   11                           5.0        1.     1000.
                        5    4   11                           5.0        1.     1000.
                        5    4   11                           5.0        1.     1000.

AREA SOLRCE CARDS
                             1.        1.     4000.       15.       .15
                            21.        1.     2CCO.       25.       .25
                            25.        1.     2000.       25.       .25
                            29.        1.     2C00.       25.       .25
                    BLANK CARD TO SIGNAL ENC OF AREA SOLRCE INVENTORY

POINT SCLRCE CARCS
                             2.        2.       10.       .10       20.       2.0       10.      32.4 STACK 1
                            14.        2.       30.       .3C       10.       2.C       15.      100. STACK 2
                             2.       16.       30.       .30       35.       1.C       12.      125. STACK 3
                    BLANK CARD TO SIGNAL ENC OF PCINT SCURCE INVENTORY
```

TABLE 14

OUTPUT LISTING FOR EXAMPLE PROBLEM 2

```
                    PEM   (VERSION  82360)


                  POLLUTION EPISODIC MODEL


                          INCLUDING
  DEPOSITION, SEDIMENTATION, AND CHEMICAL TRANSFORMATION
                        OF POLLUTANTS
```

```
                                    POLLUTION EPISODIC MODEL

INPUT CONTROL PARAMETERS:  PEM EXAMPLE 2 CHEMICAL TRANSFORMATION GAS TO PARTICLE  3-HR AVG CONCENTRATIONS

   AVERAGING TIME OPTION: NTOPT=3

         A SCENARIO IS A SET OF METEOROLOGICAL DATA FOR ONE HOUR

     1  1 HOUR: CONCENTRATIONS ARE CALCULATED FOR EACH SCENARIO
     2  24 HOURS: CONCENTRATIONS CALCULATED FOR 24 SCENARIOS ARE AVERAGED
     3  VARIABLE: CONCENTRATIONS CALCULATED FOR A GIVEN NUMBER (2 TO 24) OF SCENARIOS ARE AVERAGED

   WIND DIRECTION OPTION: NWDOPT=1

     0  DIRECTION IN DEGREES TO BE SPECIFIED FOR EACH SCENARIO
     1  SECTOR NUMBER TO BE SPECIFIED FOR EACH SCENARIO
   2-7  DIRECTION IN DEGREES TO BE SPECIFIED FOR THE FIRST OF FOUR SUB-SCENARIOS.
         FOR EACH SUCCEEDING SUB-SCENARIO, WIND DIRECTION IS AUTOMATICALLY INCREASED
         BY 90,45,30,15,10,OR 5 DEGREES, DEPENDING ON THE OPTION NUMBER SELECTED.

   WIND SPEED OPTION: NWSOPT=1

     0  SPEED IN M/S TO BE SPECIFIED FOR EACH SCENARIO
     1  WIND SPEED CLASS NUMBER TO BE SPECIFIED FOR EACH SCENARIO

   NUMBER OF SCENARIOS: NSCEN= 3

   STACK-TIP DOWNWASH ALGORITHM OPTION: NSTDWN=0

     0  ALGORITHM IS IN EFFECT
     1  ALGORITHM IS NOT USED

   RECEPTOR GRID:       COLUMNS: LX=25    ROWS: LY=25
                        SPACING: GRID=  2.000 KM
                        SOUTHWEST CORNER    XRSWC=     0.0   KM W
                                            YRSWC=     0.0   KM S

   POTENTIAL TEMPERATURE GRADIENT: DTDZ(1)=   0.020 DEG/M    STABILITY CLASS E
                                   DTDZ(2)=   0.035 DEG/M    STABILITY CLASS F
```

```
                                        POLLUTION EPISCDIC MODEL

INPUT CONTROL PARAMETERS:  PEM EXAMPLE 2 CHEMICAL TRANSFORMATION GAS TO PARTICLE  3-HR AVG CONCENTRATIONS

      NUMBER OF POLLUTANTS: NPOL=2
                                            POLLUTANT-1: GAS                    POLLUTANT-2: PARTICLE

      AREA SOURCE SCALING FACTOR:               ASCALE=     1.000                   ASCALE=     1.000
      CALIBRATICN CCEFFICIENTS:            A=      0.0    B=       0.0         A=      0.0    B=       0.0
      CALIBRATICN ICENTIFICATION:
      DEPCSITION VELOCITY (CM/S):                 VD1=    2.000                     VD2=    0.500
      SETTLING VELOCITY (CM/S):                    W1=    0.0                        W2=    0.250

      CHEMICAL TRANSFORMATION CPTION: ICT=1

         NPOL=2
           ICT=0  CHEMICAL TRANSFORMATICN LOSS OF POLLUTANTS IS IGNORED
           ICT=1  FIRST-ORDER CHEMICAL TRANSFORMATION OF POLLUTANT-1 TO POLLUTANT-2 IS CONSIDERED

      CHEMICAL TRANSFORMATION RATE: XKT= 20.000 PERCENT/HR

      RATIO OF MCLECULAR WEIGHTS OF POLLUTANT-2 (PRODUCT) TO POLLUTANT-1 (REACTANT): GAMMA= 1.500


     CUTPLT OPTICNS SELECTED:

         NARRAY=2  MAPS OF CONCENTRATION AND SURFACE DEPCSITICN FLUX AT EACH RECEPTOR IN THE GRID,
                    UNCALIBRATED ONLY
         NMAX=1     LIST OF RECEPTORS WITH HIGHEST CONCENTRATION AND SURFACE DEPOSITION FLUX
                     FOR EACH SCENARIO - PRINTED AT END OF RUN
```

```
                                        POLLUTION EPISODIC MODEL

INPUT SCENARIO PARAMETERS:  PEM EXAMPLE 2 CHEMICAL TRANSFORMATION GAS TO PARTICLE  3-HR AVG CONCENTRATIONS
                    WIND DIRECTIONS
                                                            WIND SPEED CLASSES               STABILITY CLASSES
   SECTOR    DIRECTION       SECTOR    DIRECTION
   NUMBER        (DEG)       NUMBER        (DEG)     CLASS   SPEED    CLASS                  CLASS
                                                     INDEX   (M/S)   INTERVAL(KT)            INDEX    CLASS
     1    N        0.0          9   S      180.0
     2    NNE     22.5         10   SSW    202.5
     3    NE      45.0         11   SW     225.0       1      1.50      0-3
     4    ENE     67.5         12   WSW    247.5       2      2.46      4-6                    1       A
     5    E       90.0         13   W      270.0       3      4.47       7-10                  2       B
     6    ESE    112.5         14   WNW    292.5       4      6.93      11-16                  3       C
     7    SE     135.0         15   NW     315.0       5      9.61      17-21                  4       DD (DAY)
     8    SSE    157.5         16   NNW    337.5       6     12.52    OVER 21                  5       DN (NIGHT)
                                                                                              6       E
                                                                                              7       F

SCENARIO   STABILITY   WIND SPEED     WIND       WIND      WIND        AMBIENT         INVERSION          MIXING
 NUMBER      CLASS       CLASS        SPEED     SECTOR   DIRECTION   TEMPERATURE   PENETRATION FACTOR    HEIGHT
                                      (M/S)                (DEG)       (DEG C)                            (M)

   1          DN           4          6.930       11      225.00        5.00            1.000           1000.0
   2          DN           4          6.930       11      225.00        5.00            1.000           1000.0
   3          DN           4          6.930       11      225.00        5.00            1.000           1000.0
```

```
                                   POLLUTION EPISODIC MODEL

INPUT AREA SOURCE PARAMETERS:  PEM EXAMPLE 2 CHEMICAL TRANSFORMATION GAS TO PARTICLE  3-HR AVG CONCENTRATIONS

                                                              POLLUTANT-1                  POLLUTANT-2
AREA SOURCE       COORDINATES        LENGTH OF SIDE          EMISSION RATE                EMISSION RATE
  NUMBER        X(KM)     Y(KM)           (M)            INPUT (G/S)    SCALED        INPUT (G/S)    SCALED

    1            1.00      1.00         4000.00             15.00        15.00            0.15         0.15
    2           21.00      1.00         2C00.00             25.00        25.00            0.25         0.25
    3           25.00      1.00         2000.00             25.00        25.00            0.25         0.25
    4           29.00      1.00         2000.00             25.00        25.00            0.25         0.25

 SUMS OF THE AREA SOURCE EMISSION RATES IN THIS RUN         90.00        90.00            0.90         0.90
```

```
                                        POLLUTION EPISODIC MODEL

INPUT POINT SOURCE PARAMETERS:  PEM EXAMPLE 2 CHEMICAL TRANSFORMATION GAS TO PARTICLE  3-HR AVG CONCENTRATIONS

 POINT  SOURCE            COORDINATES          EMISSION RATE        EMISSION RATE      HEIGHT    DIAMETER     EXIT VEL      EXIT TEMP
NUMBER   LABEL          X(KM)      Y(KM)     POLLUTANT-1 (G/S)    POLLUTANT-2 (G/S)     (M)        (M)          (M/S)        (DEG C)

   1     STACK 1         2.00       2.00          10.00                 0.10            20.00      2.000        10.000         32.400
   2     STACK 2        14.00       2.00          30.00                 0.30            10.00      2.000        15.000        100.000
   3     STACK 3         2.00      16.00          30.00                 0.30            35.00      1.000        12.000        125.000

 SUMS OF THE POINT SOURCE EMISSION RATES          70.00 G/S             0.70 G/S
```

```
PEM OUTPUT:  SECTICN 1 OF 1, SCENARIO  3  PEM EXAMPLE 2 CHEMICAL TRANSFORMATION GAS TO PARTICLE  3-HR AVG CONCENTRATICNS
STABILITY=DN, WIND SPD= 6.93 M/S, WIND DIR=225.00 DEG, MIXING HT= 1000.0 M, AVERAGING TIME=  3 HR.      POLLUTANT-1: GAS
UNCALIBRATEC CONCENTRATION - MICROGRAMS PER CUBIC METER

            0.0    4.00   8.00  12.00  16.00  20.00  24.00  28.00  32.00  36.00  40.00  44.00  48.00
  48.00      C  0  0  0  0  0  C  0  0  0  0  0  0  0  0  0  1  1  1  0  0  0  0  0  0      48.00
  46.00      C  0  0  0  0  0  0  0  0  0  0  0  0  0  0  1  1  1  0  0  0  0  0  0  0      46.00
  44.00      C  0  0  0  0  0  C  0  0  0  0  0  0  0  1  1  1  0  0  0  0  0  0  0  0      44.00
  42.00      0  0  0  0  0  0  C  0  0  0  0  0  0  1  1  1  0  0  0  0  0  0  0  0  0      42.00
  40.00      C  0  0  0  0  0  C  0  0  0  0  0  1  2  1  0  0  0  0  0  0  0  0  0  0      40.00
  38.CC      C  0  0  0  0  0  C  0  0  0  0  1  2  1  0  0  0  0  0  0  0  0  0  0  1      38.00
  36.00      0  0  0  0  0  0  C  0  0  0  1  2  1  0  0  0  0  0  0  0  0  0  0  1  1      36.00
  34.00      C  0  0  0  0  0  C  C  0  1  3  1  0  0  0  0  0  0  0  0  0  0  1  1  1      34.00
  32.00      C  0  0  0  0  0  C  0  2  3  1  0  0  0  0  0  0  0  0  0  0  1  1  1  0      32.00
  30.00      C  0  0  0  0  0  C  2  4  2  0  0  0  0  0  0  0  0  0  0  1  1  1  0  0      30.00
  28.0C      0  0  0  0  0  0  1  5  2  0  0  0  0  0  0  0  0  0  0  1  1  1  0  0  0      28.00
  26.00      0  0  0  0  0  1  7  1  0  0  0  0  0  1  0  0  0  0  1  2  1  0  0  0  0      26.00
  24.00      C  0  0  0  1 10  1  0  0  0  0  0  1  0  0  0  0  1  2  1  0  0  0  0  0      24.00
  22.00      C  0  0  0 16  1  0  0  0  0  0  1  0  0  0  0  1  2  1  0  0  0  0  0  0      22.00
  20.0C      0  0  0 28  0  0  C  C  0  0  1  0  0  0  0  2  3  1  0  0  0  0  0  0  0      20.00
  18.0C      C  0 60  0  0  0  C  0  1  1  0  0  0  0  2  4  2  0  0  0  0  0  0  0  0      18.00
  16.00      C  0  0  0  C  0  0  1  1  1  0  0  0  2  5  2  0  0  0  0  0  0  0  0  0      16.00
  14.00      C  0  0  0  0  0  C  2  1  0  0  0  2  6  2  0  0  0  0  0  0  0  0  0  0      14.00
  12.00      C  0  0  0  0  1  3  0  0  0  0  1  8  2  0  0  0  0  0  0  0  0  0  0  0      12.00
  10.00      C  0  0  0  1  5  1  0  0  0  1 12  1  0  0  4  0  4  0  4  0  0  0  0  0      10.00
   8.00      C  0  0  1  8  1  C  0  0  0 17  1  0  0  5  0  5  0  5  0  0  0  0  0  0       8.00
   6.00      C  0  2 15  1  0  0  0  0 30  0  0  0  7  0  7  0  7  0  0  0  0  0  0  0       6.00
   4.00      C 10 43  2  0  0  0  0 55  0  0  0 14  0 14  0 14  0  0  0  0  0  0  0  0       4.00
   2.00      0 10 10  0  0  0  C  0  0  0  0 65  0 65  0 65  0  0  0  0  0  0  0  0  0       2.00
   0.0       0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0       0.0
            0.0    4.00   8.00  12.00  16.00  20.00  24.00  28.00  32.00  36.00  40.00  44.00  48.00
```

```
PEM OUTPUT:  SECTION 1 OF 1, SCENARIO  3  PEM EXAMPLE 2 CHEMICAL TRANSFORMATION GAS TO PARTICLE  3-HR AVG CONCENTRATIONS
STABILITY=DN, WIND SPD= 6.93 M/S, WIND DIR=225.00 DEG, MIXING HT= 1000.0 M, AVERAGING TIME=  3 HR.       POLLUTANT-1: GAS
UNCALIBRATED SURFACE DEPOSITION FLUX - KILOGRAMS PER SQUARE KILOMETER PER HOUR

           0.0    4.00    8.00   12.00   16.00   20.00   24.00   28.00   32.00   36.00   40.00   44.00   48.00
   48.00     0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0     48.00
   46.00     0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0     46.00
   44.00     0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0     44.00
   42.00     0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0     42.00
   40.00     0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0     40.00
   38.00     0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0     38.00
   36.00     0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0     36.00
   34.00     0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0     34.00
   32.00     0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0     32.00
   30.00     0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0     30.00
   28.00     0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0     28.00
   26.00     0   0   0   0   0   0   1   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0     26.00
   24.00     0   0   0   0   0   1   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0     24.00
   22.00     0   0   0   0   1   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0     22.00
   20.00     0   0   0   2   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0     20.00
   18.00     0   0   4   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0     18.00
   16.00     0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0     16.00
   14.00     0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0     14.00
   12.00     0   0   0   0   0   0   0   0   0   0   0   0   1   0   0   0   0   0   0   0   0   0   0   0   0     12.00
   10.00     0   0   0   0   0   0   0   0   0   0   0   1   0   0   0   0   0   0   0   0   0   0   0   0   0     10.00
    8.00     0   0   0   0   1   0   0   0   0   0   1   0   0   0   0   0   0   0   0   0   0   0   0   0   0      8.00
    6.00     0   0   0   1   0   0   0   0   0   2   0   0   0   1   0   1   0   1   0   0   0   0   0   0   0      6.00
    4.00     0   1   3   0   0   0   0   0   4   0   0   0   1   0   1   0   1   0   0   0   0   0   0   0   0      4.00
    2.00     0   1   1   0   0   0   0   0   0   0   0   5   0   5   0   5   0   0   0   0   0   0   0   0   0      2.00
     0.0     0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0       0.0
           0.0    4.00    8.00   12.00   16.00   20.00   24.00   28.00   32.00   36.00   40.00   44.00   48.00
```

```
PEM OUTPUT:  SECTION 1 OF 1, SCENARIO  3  PEM EXAMPLE 2 CHEMICAL TRANSFORMATION GAS TO PARTICLE  3-HR AVG CONCENTRATIONS
STABILITY=DN, WIND SPD= 6.93 M/S, WIND DIR=225.00 DEG, MIXING HT= 1000.0 M, AVERAGING TIME=  3 HR.      POLLUTANT-2: PARTICLE
UNCALIBRATED CONCENTRATION - MICROGRAMS PER CUBIC METER

             0.0     4.00    8.00    12.00   16.00   20.00   24.00   28.00   32.00   36.00   40.00   44.00   48.00
   48.00     0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   1   1   1   0   0   0   0   0   0      48.00
   46.00     0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   1   1   1   0   0   0   0   0   0   0      46.00
   44.00     0   0   0   0   0   0   0   0   0   0   0   0   0   0   1   1   1   0   0   0   0   0   0   0   0      44.00
   42.00     0   0   0   0   0   0   0   0   0   0   0   0   0   1   1   1   0   0   0   0   0   0   0   0   0      42.00
   40.00     0   0   0   0   0   0   0   0   0   0   0   0   1   1   1   0   0   0   0   0   0   0   0   0   0      40.00
   38.00     0   0   0   0   0   0   0   0   0   0   0   1   1   1   0   0   0   0   0   0   0   0   0   0   0      38.00
   36.00     0   0   0   0   0   0   0   0   0   0   1   1   1   0   0   0   0   0   0   0   0   0   0   0   1      36.00
   34.00     0   0   0   0   0   0   0   0   0   1   1   1   0   0   0   0   0   0   0   0   0   0   0   1   1      34.00
   32.00     0   0   0   0   0   0   0   0   0   1   1   0   0   0   0   0   0   0   0   0   0   0   1   1   1      32.00
   30.00     0   0   0   0   0   0   0   0   1   0   0   0   0   0   0   0   0   0   0   0   0   1   1   1   0      30.00
   28.00     0   0   0   0   0   0   0   1   0   0   0   0   0   0   0   0   0   0   0   0   1   1   1   0   0      28.00
   26.00     0   0   0   0   0   0   1   0   0   0   0   0   0   0   0   0   0   0   1   1   1   0   0   0   0      26.00
   24.00     0   0   0   0   0   2   0   0   0   0   0   0   0   0   0   0   0   1   1   1   0   0   0   0   0      24.00
   22.00     0   0   0   0   2   0   0   0   0   0   0   0   0   0   0   0   1   2   1   0   0   0   0   0   0      22.00
   20.00     0   0   0   2   0   0   0   0   0   0   0   0   0   0   0   1   2   1   0   0   0   0   0   0   0      20.00
   18.00     0   0   2   0   0   0   0   0   0   0   0   0   0   0   1   2   1   0   0   0   0   0   0   0   0      18.00
   16.00     0   0   0   0   0   0   0   0   0   0   0   0   0   1   2   1   0   0   0   0   0   0   0   0   0      16.00
   14.00     0   0   0   0   0   0   0   1   0   0   0   0   0   2   1   0   0   0   0   0   0   0   0   0   0      14.00
   12.00     0   0   0   0   0   0   1   0   0   0   0   0   2   0   0   0   0   0   0   0   0   0   0   0   0      12.00
   10.00     0   0   0   0   0   1   0   0   0   0   0   3   0   0   0   0   0   0   0   0   0   0   0   0   0      10.00
    8.00     0   0   0   0   1   0   0   0   0   0   3   0   0   0   0   0   0   0   0   0   0   0   0   0   0       8.00
    6.00     0   0   0   1   0   0   0   0   0   3   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0       6.00
    4.00     0   0   2   0   0   0   0   0   3   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0       4.00
    2.00     0   0   0   0   0   0   0   0   0   0   0   1   0   1   0   1   0   0   0   0   0   0   0   0   0       2.00
    0.0      0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0       0.0
             0.0     4.00    8.00    12.00   16.00   20.00   24.00   28.00   32.00   36.00   40.00   44.00   48.00
```

```
PEM OUTPUT:  SECTION 1 OF 1, SCENARIO  3  PEM EXAMPLE 2 CHEMICAL TRANSFORMATION GAS TO PARTICLE  3-HR AVG CONCENTRATIONS
STABILITY=DN, WIND SPD= 6.93 M/S, WIND DIR=225.00 DEG, MIXING HT= 1000.0 M, AVERAGING TIME=  3 HR.      POLLUTANT-2: PARTICLE
UNCALIBRATED SURFACE DEPOSITION FLUX - MICROGRAMS PER SQUARE METER PER HOUR

             0.0    4.00    8.00   12.00   16.00   20.00   24.00   28.00   32.00   36.00   40.00   44.00   48.00
   48.00       0   0   0   0   0   0   0   0   0   0   0   0   0   0   1   5  10  13  10   5   2   1   0   0   0      48.00
   46.00       0   0   0   0   0   0   0   0   0   0   0   0   0   1   4  10  13  10   5   2   1   2   0   0   0      46.00
   44.00       0   0   0   0   0   0   0   0   0   0   0   0   1   4  10  14  10   5   2   1   2   3   4   0   1      44.00
   42.00       0   0   0   0   0   0   0   0   0   0   0   0   3  10  15  10   4   1   1   2   4   4   4   3   3      42.00
   40.00       0   0   0   0   0   0   0   0   0   0   0   3  10  15  10   4   1   1   2   4   4   4   3   4   9      40.00
   38.00       0   0   0   0   0   0   0   0   0   0   2  10  16  10   3   1   1   2   4   4   4   3   4   9  16      38.00
   36.00       0   0   0   0   0   0   0   0   0   1  10  17  10   3   0   1   2   4   5   4   2   3   8  16  20      36.00
   34.00       0   0   0   0   0   0   0   0   1   9  18  10   2   0   0   2   4   5   4   2   2   8  16  20  16      34.00
   32.00       0   0   0   0   0   0   0   0   8  20   9   1   0   0   2   4   5   4   2   2   7  17  22  16   8      32.00
   30.00       0   0   0   0   0   0   0   7  21   8   1   0   0   1   4   5   4   2   1   6  17  23  17   7   2      30.00
   28.00       0   0   0   0   0   0   5  23   7   0   0   0   1   4   6   4   2   1   5  17  24  17   7   2   0      28.00
   26.00       0   0   0   0   0   3  25   5   0   0   0   1   4   6   4   1   1   4  17  25  17   6   1   0   0      26.00
   24.00       0   0   0   0   1  28   3   0   0   0   1   4   6   4   1   0   3  17  27  17   5   1   0   0   0      24.00
   22.00       0   0   0   0  31   1   0   0   0   1   4   7   4   1   0   2  16  28  17   4   1   0   0   0   0      22.00
   20.00       0   0   0  37   0   0   0   0   0   4   7   4   1   0   1  15  30  16   3   0   0   0   0   0   0      20.00
   18.00       0   0  44   0   0   0   0   0   3   8   4   1   0   1  14  33  15   2   0   0   0   0   0   0   0      18.00
   16.00       0   0   0   0   0   0   0   3   9   3   0   0   0  12  35  14   1   0   0   0   0   0   0   0   0      16.00
   14.00       0   0   0   0   0   0   2  10   3   0   0   0   9  38  12   1   0   0   0   0   0   0   0   0   0      14.00
   12.00       0   0   0   0   0   2  11   2   0   0   0   5  41   9   0   0   0   0   0   0   0   0   0   0   0      12.00
   10.00       0   0   0   0   1  13   2   0   0   0   2  45   5   0   0   1   0   1   0   1   0   0   0   0   0      10.00
    8.00       0   0   0   0  15   1   0   0   0   0  49   2   0   0   2   0   2   0   2   0   0   0   0   0   0       8.00
    6.00       0   0   1  18   0   0   0   0   0  55   0   0   0   2   0   2   0   2   0   0   0   0   0   0   0       6.00
    4.00       0   2  28   1   0   0   0   0  53   0   0   0   3   0   3   0   3   0   0   0   0   0   0   0   0       4.00
    2.00       0   2   2   0   0   0   0   0   0   0   0  13   0  13   0  13   0   0   0   0   0   0   0   0   0       2.00
     0.0       0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0        0.0
             0.0    4.00    8.00   12.00   16.00   20.00   24.00   28.00   32.00   36.00   40.00   44.00   48.00
```

```
                              POLLUTION EPISODIC MODEL

  OUTPUT:  PEM EXAMPLE 2 CHEMICAL TRANSFORMATION GAS TO PARTICLE  3-HR AVG CONCENTRATIONS

  HIGHEST PREDICTEC CCNCENTRATICN OF EACH PULLUTANT FOR EACH SCENARIO

  UNCALIBRATED CONCENTRATION IN MICROGRAMS PER CUBIC METER  -  CALIBRATION, POLLUTANT-1:
                                                               CALIBRATION, POLLUTANT-2:

                                  POLLUTANT-1: GAS                                  POLLUTANT-2: PARTICLE
SCENARIO  WIND DIRECTION     CCORDINATES           CONCENTRATION             CCORDINATES          CONCENTRATICN
 NUMBER    SUB-SCENARIC    X(KM)     Y(KM)    UNCALIBRATED   CALIBRATED    X(KM)     Y(KM)    UNCALIBRATED   CALIBRATED

    1           1          30.00     2.C0        65.0452         0.0        18.00     6.00       3.0750          0.0
```

```
                              POLLUTION EPISCDIC MODEL

   OUTPUT:  PEM EXAMPLE 2 CHEMICAL TRANSFORMATICN GAS TO PARTICLE  3-HR AVG CONCENTRATIONS

   HIGHEST PREDICTED SURFACE DEPOSITION FLUX OF EACH POLLUTANT FOR EACH SCENARIO

   UNCALIBRATED VALUES IN MICROGRAMS PER SQLARE METER PER HOUR  -  CALIBRATION, POLLUTANT-1:
                                                                   CALIBRATICN, POLLUTANT-2:

                                  POLLUTANT-1: GAS                                              POLLUTANT-2: PARTICLE
SCENARIO  WINC DIRECTICN        COORDINATES          SURFACE DEPOSITION FLUX            COORDINATES          SURFACE DEPOSITICN FLUX
 NUMBER     SUB-SCENARIO      X(KM)     Y(KM)     UNCALIBRATED     CALIBRATED         X(KM)     Y(KM)     UNCALIBRATED     CALIBRATED

    1            1            30.00      2.00      4683.2500          0.0             18.00      6.00       55.3507           0.0
IHC002I STOP     0
```

TABLE 15

INPUT DATA FOR EXAMPLE PROBLEM 3

```
                                           CARD IMAGES
CONTROL CARDS
  1  TITLE         PEM EXAMPLE 3   CHEMICAL TRANSFORMATION GAS TO PARTICLE  6-HR AVG CONCENTRATION
  2  OPTIONS          3    0    0    6    0    2    0    0    1    1    0    1    0
  3  GRID                0.0          0.0         25          25          4.0         0.0         0.0
  4  POLLUTANTS       2    1          1.0         0.0         2.0         1.0        10.0         1.5
  5  SCALING             1.0          1.0         0.0         0.0         0.0         0.0
  6  LABELS        GAS                                                PARTICLE
SCENARIO CARDS

                      7    0    0        2.0    270.0     5.0      1.0    200.0
                      7    0    0        2.5    270.0     3.0      1.0    200.0
                      7    0    0        2.0    270.0     1.0      1.0    175.0
                      7    0    0        2.5    270.0    -1.0      1.0    175.0
                      7    0    0        2.0    270.0    -3.0      1.0    150.0
                      7    0    0        2.5    270.0    -5.0      1.0    150.0
AREA SOURCE CARDS

                        6.0      18.0    20000.     250.0       2.5
                   BLANK CARD TO SIGNAL END OF AREA SOURCE INVENTORY
POINT SOURCE CARDS

                       16.0      8.0     10.0     0.0     10.0    0.50     1.0    60.0STACK AR
                        4.0     48.0     12.5     0.0     15.0    0.75     2.0    70.0STACK AS
                       48.0     28.0     20.0     0.0     30.0    1.00     3.0    80.0STACK AT
                   BLANK CARD TO SIGNAL END OF POINT SOURCE INVENTORY
```

TABLE 16

OUTPUT LISTING FOR EXAMPLE PROBLEM 3

```
                    PEM   (VERSION  82360)


                 PCLLUTION EPISODIC MODEL


                        INCLUDING
DEPCSITIUN, SECIMENTATIUN, AND CHEMICAL TRANSFORMATICN
                      UF PULLUTANTS
```

```
                                        POLLUTION EPISODIC MODEL

INPUT CONTROL PARAMETERS:  PEM EXAMPLE 3   CHEMICAL TRANSFORMATION GAS TO PARTICLE  6-HR AVG CONCENTRATION

     AVERAGING TIME OPTION: NTOPT=3

            A SCENARIO IS A SET OF METEOROLOGICAL DATA FOR ONE HOUR

       1  1 HOUR: CONCENTRATIONS ARE CALCULATED FOR EACH SCENARIO
       2  24 HOURS: CONCENTRATIONS CALCULATED FOR 24 SCENARIOS ARE AVERAGED
       3  VARIABLE: CONCENTRATIONS CALCULATED FOR A GIVEN NUMBER (2 TO 24) OF SCENARIOS ARE AVERAGED

     WIND DIRECTION OPTION: NWDOPT=0

       0  DIRECTION IN DEGREES TO BE SPECIFIED FOR EACH SCENARIO
       1  SECTOR NUMBER TO BE SPECIFIED FOR EACH SCENARIO
     2-7  DIRECTION IN DEGREES TO BE SPECIFIED FOR THE FIRST OF FOUR SUB-SCENARIOS.
            FOR EACH SUCCEEDING SUB-SCENARIO, WIND DIRECTION IS AUTOMATICALLY INCREASED
            BY 90,45,30,15,10,OR 5 DEGREES, DEPENDING ON THE OPTION NUMBER SELECTED.

     WIND SPEED OPTION: NWSOPT=0

       0  SPEED IN M/S TO BE SPECIFIED FOR EACH SCENARIO
       1  WIND SPEED CLASS NUMBER TO BE SPECIFIED FOR EACH SCENARIO

     NUMBER OF SCENARIOS: NSCEN= 6

     STACK-TIP DOWNWASH ALGORITHM OPTION: NSTDWN=1

       0  ALGORITHM IS IN EFFECT
       1  ALGORITHM IS NOT USED

     RECEPTOR GRID:          COLUMNS: LX=25    ROWS: LY=25
                             SPACING: GRID=  4.000 KM
                             SOUTHWEST CORNER     XRSWC=     0.0   KM W
                                                  YRSWC=     0.0   KM S

     POTENTIAL TEMPERATURE GRADIENT: DTDZ(1)=   0.020 DEG/M    STABILITY CLASS E
                                     DTDZ(2)=   0.035 DEG/M    STABILITY CLASS F
```

```
                                          POLLUTION EPISODIC MODEL

INPUT CONTROL PARAMETERS:  PEM EXAMPLE 3   CHEMICAL TRANSFORMATION GAS TO PARTICLE  6-HR AVG CONCENTRATION

      NUMBER OF POLLUTANTS: NPOL=2
                                              POLLUTANT-1: GAS                  POLLUTANT-2: PARTICLE

      AREA SOURCE SCALING FACTOR:               ASCALE=    1.000                  ASCALE=    1.000
      CALIBRATION COEFFICIENTS:               A=     0.0    B=     0.0          A=     0.0    B=     0.0
      CALIBRATION IDENTIFICATION:
      DEPOSITION VELOCITY (CM/S):                  VD1=   1.000                    VD2=   2.000
      SETTLING VELOCITY (CM/S):                     W1=   0.0                       W2=   1.000

      CHEMICAL TRANSFORMATION OPTION: ICT=1

         NPOL=2
           ICT=0  CHEMICAL TRANSFORMATION LOSS OF POLLUTANTS IS IGNORED
           ICT=1  FIRST-ORDER CHEMICAL TRANSFORMATION OF POLLUTANT-1 TO POLLUTANT-2 IS CONSIDERED

      CHEMICAL TRANSFORMATION RATE: XKT= 10.000 PERCENT/HR

      RATIO OF MOLECULAR WEIGHTS OF POLLUTANT-2 (PRODUCT) TO POLLUTANT-1 (REACTANT): GAMMA= 1.500


     OUTPUT OPTIONS SELECTED:

         NARRAY=2  MAPS OF CONCENTRATION AND SURFACE DEPOSITION FLUX AT EACH RECEPTOR IN THE GRID,
                    UNCALIBRATED ONLY
         NPRINT=1  LIST OF POINT SOURCE PARAMETERS AND EFFECTIVE STACK HEIGHTS
                    PRINTED AT BEGINNING OF EACH SCENARIO
         NMAX=1    LIST OF RECEPTORS WITH HIGHEST CONCENTRATION AND SURFACE DEPOSITION FLUX
                    FOR EACH SCENARIO - PRINTED AT END OF RUN
```

```
                                    POLLUTION EPISODIC MODEL

INPUT SCENARIC PARAMETERS:  PEM EXAMPLE 3   CHEMICAL TRANSFORMATION GAS TO PARTICLE  6-HR AVG CONCENTRATION

                    WIND DIRECTIONS                               WIND SPEED CLASSES              STABILITY CLASSES

     SECTOR     DIRECTION          SECTOR     DIRECTION        CLASS    SPEED    CLASS
     NUMBER         (DEG)          NUMBER         (DEG)        INDEX    (M/S)    INTERVAL(KT)         CLASS
                                                                                                      INDEX    CLASS
        1    N        0.0             9    S      180.0
        2    NNE     22.5            10    SSW    202.5          1       1.50       0-3                  1       A
        3    NE      45.0            11    SW     225.0          2       2.46       4-6                  2       B
        4    ENE     67.5            12    WSW    247.5          3       4.47       7-10                 3       C
        5    E       90.0            13    W      270.0          4       6.93      11-16                 4       DD (DAY)
        6    ESE    112.5            14    WNW    292.5          5       9.61      17-21                 5       DN (NIGHT)
        7    SE     135.0            15    NW     315.0          6      12.52     OVER 21                6       E
        8    SSE    157.5            16    NNW    337.5                                                7       F

 SCENARIO   STABILITY   WIND SPEED    WIND         WIND      WIND        AMBIENT          INVERSION           MIXING
  NUMBER      CLASS       CLASS       SPEED        SECTOR    DIRECTION   TEMPERATURE   PENETRATION FACTOR     HEIGHT
                                      (M/S)                  (DEG)       (DEG C)                              (M)

     1          F                     2.000                  270.00         5.00            1.000             200.0
     2          F                     2.500                  270.00         3.00            1.000             200.0
     3          F                     2.000                  270.00         1.00            1.000             175.0
     4          F                     2.500                  270.00        -1.00            1.000             175.0
     5          F                     2.000                  270.00        -3.00            1.000             150.0
     6          F                     2.500                  270.00        -5.00            1.000             150.0
```

```
                                        POLLUTION EPISODIC MODEL

INPUT AREA SOURCE PARAMETERS:  PEM EXAMPLE 3   CHEMICAL TRANSFORMATION GAS TO PARTICLE  6-HR AVG CONCENTRATION

AREA SOURCE        COORDINATES          LENGTH OF SIDE           POLLUTANT-1                  POLLUTANT-2
  NUMBER         X(KM)     Y(KM)             (M)               EMISSION RATE                EMISSION RATE
                                                           INPUT (G/S)    SCALED        INPUT (G/S)    SCALED
     1            6.00     18.00          20000.00          250.000      250.000           2.500        2.500

 SUMS OF THE AREA SOURCE EMISSION RATES IN THIS RUN          250.000      250.000           2.500        2.500
```

```
                              POLLUTION EPISODIC MODEL

INPUT POINT SOURCE PARAMETERS:  PEM EXAMPLE 3   CHEMICAL TRANSFORMATION GAS TO PARTICLE  6-HR AVG CONCENTRATION

 POINT SOURCE         COORDINATES       EMISSION RATE      EMISSION RATE     HEIGHT    DIAMETER    EXIT VEL     EXIT TEMP
NUMBER   LABEL       X(KM)    Y(KM)   POLLUTANT-1 (G/S)  POLLUTANT-2 (G/S)    (M)        (M)        (M/S)        (DEG C)

   1    STACK AR     16.00     8.00        10.000              0.0           10.00      0.500       1.000        60.000
   2    STACK AS      4.00    48.00        12.500              0.0           15.00      0.750       2.000        70.000
   3    STACK AT     40.00    28.00        20.000              0.0           30.00      1.000       3.000        80.000

 SUMS OF THE POINT SOURCE EMISSION RATES       42.500 G/S          0.0   G/S
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                                        POLLUTION EPISODIC MODEL

    OUTPUT:  PEM EXAMPLE 3   CHEMICAL TRANSFORMATION GAS TO PARTICLE  6-HR AVG CONCENTRATION

    SCENARIO 1    POINT SOURCE PLUME RISE CALCULATIONS
                    MIXING HEIGHT: HMIX= 200.00 M
                   IF MAXIMUM EFFECTIVE SOURCE HEIGHT IS GREATER THAN   200.0 M, THE SOURCE IS IGNORED

             SOURCE          EMISSION RATES
POINT     COORDINATES       POL-1      POL-2                                                          WIND SPEED AT    MAXIMUM
SOURCE   X(KM)    Y(KM)     (G/S)      (G/S)     HEIGHT  DIAMETER  EXIT VEL  EXIT TEMP   DOMINANT     STACK HEIGHT    EFFECTIVE
                                                  (M)      (M)      (M/S)    (DEG K)    INFLUENCE       (M/S)     SOURCE HEIGHT(M)

   1     16.00     8.00     10.00       0.0      10.00    0.500     1.000    333.15  BUOYANCY          2.000           18.97
   2      4.00    48.00     12.50       0.0      15.00    0.750     2.000    343.15  BUOYANCY          2.259           29.88
   3     48.00    28.00     20.00       0.0      30.00    1.000     3.000    353.15  BUOYANCY          2.781           50.00
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                                        POLLUTION EPISODIC MODEL

        OUTPUT:  PEM EXAMPLE 3   CHEMICAL TRANSFORMATION GAS TO PARTICLE  6-HR AVG CONCENTRATION

        SCENARIO 2    POINT SOURCE PLUME RISE CALCULATIONS
                         MIXING HEIGHT: HMIX= 200.00 M
                         IF MAXIMUM EFFECTIVE SOURCE HEIGHT IS GREATER THAN   200.0 M, THE SOURCE IS IGNORED

                   SOURCE          EMISSION RATES
  POINT         COORDINATES        POL-1      POL-2      HEIGHT  DIAMETER  EXIT VEL  EXIT TEMP    DOMINANT    WIND SPEED AT     MAXIMUM
  SOURCE     X(KM)     Y(KM)       (G/S)      (G/S)       (M)      (M)      (M/S)    (DEG K)     INFLUENCE    STACK HEIGHT     EFFECTIVE
                                                                                                                (M/S)      SOURCE HEIGHT(M)
    1        16.00      8.00       10.00       0.0       10.00    0.500     1.000     333.15  BUOYANCY          2.500           18.40
    2         4.00     48.00       12.50       0.0       15.00    0.750     2.000     343.15  BUOYANCY          2.823           28.92
    3        48.00     28.00       20.00       0.0       30.00    1.000     3.000     353.15  BUOYANCY          3.476           48.69
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                                  POLLUTION EPISODIC MODEL

   OUTPUT:  PEM EXAMPLE 3   CHEMICAL TRANSFCRMATION GAS TO PARTICLE  6-HR AVG CONCENTRATION

   SCENARIO 3    PCINT SOURCE PLUME RISE CALCULATICNS
                    MIXING HEIGHT: HMIX= 175.CO M
                    IF MAXIMUM EFFECTIVE SOURCE HEIGHT IS GREATER THAN   175.0 M, THE SOURCE IS IGNORED

                SOURCE          EMISSION RATES                                                                  WIND SPEED AT    MAXIMUM
  PCINT      CCORDINATES       POL-1       POL-2      HEIGHT  DIAMETER  EXIT VEL  EXIT TEMP      DOMINANT      STACK HEIGHT    EFFECTIVE
  SOURCE   X(KM)     Y(KM)     (G/S)       (G/S)       (M)      (M)      (M/S)     (DEG K)       INFLUENCE         (M/S)      SOURCE HEIGHT(M)

     1     16.00      8.00     10.00        0.0       10.00    0.500     1.000     333.15  BUOYANCY              2.000            19.13
     2      4.CO     48.0C     12.50        0.0       15.00    0.750     2.000     343.15  BUOYANCY              2.259            30.11
     3     48.CO     28.0C     20.00        0.0       30.00    1.000     3.000     353.15  BUOYANCY              2.781            50.25
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                                    POLLUTION EPISODIC MODEL

   OUTPUT:  PEM EXAMPLE 3   CHEMICAL TRANSFORMATION GAS TO PARTICLE  6-HR AVG CONCENTRATION

   SCENARIO 4    POINT SOURCE PLUME RISE CALCULATIONS
                    MIXING HEIGHT: HMIX= 175.00 M
                    IF MAXIMUM EFFECTIVE SOURCE HEIGHT IS GREATER THAN   175.0 M, THE SOURCE IS IGNORED

                  SOURCE          EMISSION RATES                                                                WIND SPEED AT    MAXIMUM
 POINT         COORDINATES       POL-1       POL-2       HEIGHT  DIAMETER   EXIT VEL  EXIT TEMP      DOMINANT     STACK HEIGHT     EFFECTIVE
 SOURCE     X(KM)     Y(KM)     (G/S)       (G/S)        (M)      (M)        (M/S)    (DEG K)       INFLUENCE       (M/S)      SOURCE HEIGHT(M)

    1       16.00      8.00     10.00        0.0        10.00    0.500       1.000    333.15  BUOYANCY              2.500            18.55
    2        4.00     48.00     12.50        0.0        15.00    0.750       2.000    343.15  BUOYANCY              2.823            29.12
    3       48.00     28.00     20.00        0.0        30.00    1.000       3.000    353.15  BUOYANCY              3.476            48.91
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                                        POLLUTION EPISODIC MODEL

     OUTPUT:  PEM EXAMPLE 3   CHEMICAL TRANSFORMATION GAS TO PARTICLE  6-HR AVG CONCENTRATION

     SCENARIO 5    POINT SOURCE PLUME RISE CALCULATIONS
                      MIXING HEIGHT: HMIX= 150.00 M
                      IF MAXIMUM EFFECTIVE SOURCE HEIGHT IS GREATER THAN   150.0 M, THE SOURCE IS IGNORED

 POINT         SOURCE          EMISSION RATES
 SOURCE      COORDINATES      POL-1      POL-2      HEIGHT  DIAMETER  EXIT VEL  EXIT TEMP     DOMINANT      WIND SPEED AT     MAXIMUM
          X(KM)     Y(KM)     (G/S)      (G/S)       (M)      (M)      (M/S)    (DEG K)      INFLUENCE     STACK HEIGHT     EFFECTIVE
                                                                                                            (M/S)       SOURCE HEIGHT(M)
   1      16.00      8.00     10.00       0.0       10.00    0.500     1.000    333.15  BUOYANCY              2.000             19.29
   2       4.00     48.00     12.50       0.0       15.00    0.750     2.000    343.15  BUOYANCY              2.259             30.32
   3      48.00     28.00     20.00       0.0       30.00    1.000     3.000    353.15  BUOYANCY              2.781             50.49
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                                        POLLUTION EPISODIC MODEL

     OUTPUT:  PEM EXAMPLE 3   CHEMICAL TRANSFORMATION GAS TO PARTICLE  6-HR AVG CONCENTRATION

     SCENARIO 6    POINT SOURCE PLUME RISE CALCULATIONS
                     MIXING HEIGHT: HMIX= 150.00 M
                     IF MAXIMUM EFFECTIVE SOURCE HEIGHT IS GREATER THAN   150.0 M, THE SOURCE IS IGNORED

                SOURCE          EMISSION RATES
 POINT       COORDINATES       POL-1      POL-2                                                                      WIND SPEED AT     MAXIMUM
 SOURCE     X(KM)    Y(KM)     (G/S)      (G/S)     HEIGHT   DIAMETER   EXIT VEL   EXIT TEMP      DOMINANT       STACK HEIGHT     EFFECTIVE
                                                      (M)       (M)       (M/S)     (DEG K)       INFLUENCE          (M/S)      SOURCE HEIGHT(M)
   1        16.00     8.00     10.00       0.0      10.00     0.500      1.000      333.15   BUOYANCY             2.500            18.69
   2         4.00    48.00     12.50       0.0      15.00     0.750      2.000      343.15   BUOYANCY             2.823            29.31
   3        48.00    28.00     20.00       0.0      30.00     1.000      3.000      353.15   BUOYANCY             3.476            49.12
```

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PEM OUTPUT:  SECTION 1 OF 1, SCENARIO  6  PEM EXAMPLE 3   CHEMICAL TRANSFORMATION GAS TO PARTICLE  6-HR AVG CONCENTRATION
STABILITY=F , WIND SPD= 2.50 M/S, WIND DIR=270.00 DEG, MIXING HT=  150.0 M, AVERAGI[illegible]ME=  6 HR.      POLLUTANT-1: GAS
UNCALIBRATED CONCENTRATION - MICROGRAMS PER CUBIC METER

             0.0    8.00   16.00   24.00   32.00   40.00   48.00   56.00   64.00   72.00   80.00   88.00   96.00

    96.00      0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0       96.00
    92.00      0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0       92.00
    88.00      0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0       88.00
    84.00      0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0       84.00
    80.00      0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0       80.00
    76.00      0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0       76.00
    72.00      0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0       72.00
    68.00      0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0       68.00
    64.00      0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0       64.00
    60.00      0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0       60.00
    56.00      0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0       56.00
    52.00      0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0       52.00
    48.00      0   0 145  49  24  13   8   6   4   3   2   2   1   1   1   1   1   0   0   0   0   0   0   0   0       48.00
    44.00      0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0       44.00
    40.00      0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0       40.00
    36.00      0   0  60  69  72  75  76  16   7   4   1   0   0   0   0   0   0   0   0   0   0   0   0   0   0       36.00
    32.00      0   0  60  69  72  75  76  16   7   4   1   0   0   0   0   0   0   0   0   0   0   0   0   0   0       32.00
    28.00      0   0  60  69  72  75  76  16   7   4   1   0   0  96  54  31  20  14  10   7   5   4   3   3   2       28.00
    24.00      0   0  60  69  72  75  76  16   7   4   1   0   0   0   0   0   0   0   0   0   0   0   0   0   0       24.00
    20.00      0   0  60  69  72  75  76  16   7   4   1   0   0   0   0   0   0   0   0   0   0   0   0   0   0       20.00
    16.00      0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0       16.00
    12.00      0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0       12.00
     8.00      0   0   0   0   0 143  40  18   9   6   4   3   2   1   1   1   1   1   0   0   0   0   0   0   0        8.00
     4.00      0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0        4.00
      0.0      0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0         0.0

             0.0    8.00   16.00   24.00   32.00   40.00   48.00   56.00   64.00   72.00   80.00   88.00   96.00
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PEM OUTPUT:  SECTION 1 OF 1, SCENARIO  6  PEM EXAMPLE 3   CHEMICAL TRANSFORMATION GAS TO PARTICLE  6-HR AVG CONCENTRATION
STABILITY=F  , WIND SPD= 2.50 M/S, WIND DIR=270.00 DEG, MIXING HT=  150.0 M, AVERAGING TIME=  6 HR.
UNCALIBRATED SURFACE DEPOSITION FLUX - KILOGRAMS PER SQUARE KILOMETER PER HOUR                     POLLUTANT-1: GAS
              0.0      8.00     16.00     24.00     32.00     40.00     48.00     56.00     64.00     72.00     80.00     88.00     96.00
   96.00       0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0      96.00
   92.00       0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0      92.00
   88.00       0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0      88.00
   84.00       0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0      84.00
   80.00       0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0      80.00
   76.00       0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0      76.00
   72.00       0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0      72.00
   68.00       0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0      68.00
   64.00       0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0      64.00
   60.00       0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0      60.00
   56.00       0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0      56.00
   52.00       0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0      52.00
   48.00       0    0    5    2    1    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0      48.00
   44.00       0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0      44.00
   40.00       0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0      40.00
   36.00       0    0    2    2    3    3    3    1    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0      36.00
   32.00       0    0    2    2    3    3    3    1    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0      32.00
   28.00       0    0    2    2    3    3    3    1    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0      28.00
   24.00       0    0    2    2    3    3    3    1    0    0    0    0    0    3    2    1    1    0    0    0    0    0    0    0    0      24.00
   20.00       0    0    2    2    3    3    3    1    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0      20.00
   16.00       0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0      16.00
   12.00       0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0      12.00
    8.00       0    0    0    0    0    5    1    1    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0       8.00
    4.00       0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0       4.00
    0.0        0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0       0.0
              0.0      8.00     16.00     24.00     32.00     40.00     48.00     56.00     64.00     72.00     80.00     88.00     96.00
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PEM OUTPUT:  SECTION 1 OF 1, SCENARIO  6  PEM EXAMPLE 3   CHEMICAL TRANSFORMATION GAS TO PARTICLE  6-HR AVG CONCENTRATION
STABILITY=F , WIND SPD= 2.50 M/S, WIND DIR=270.00 DEG, MIXING HT=  150.0 M, AVERAGING TIME=  6 HR.      POLLUTANT-2: PARTICLE
UNCALIBRATED CONCENTRATION - MICROGRAMS PER CUBIC METER
                0.0     8.00    16.00    24.00    32.00    40.00    48.00    56.00    64.00    72.00    80.00    88.00    96.00
   96.00        0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0       96.00
   92.00        0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0       92.00
   88.00        0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0       88.00
   84.00        0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0       84.00
   80.00        0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0       80.00
   76.00        0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0       76.00
   72.00        0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0       72.00
   68.00        0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0       68.00
   64.00        0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0       64.00
   60.00        0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0       60.00
   56.00        0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0       56.00
   52.00        0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0       52.00
   48.00        0   0  12   7   4   2   2   1   1   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0       48.00
   44.00        0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0       44.00
   40.00        0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0       40.00
   36.00        0   0   1   3   4   5   6   5   3   2   1   0   0   0   0   0   0   0   0   0   0   0   0   0   0       36.00
   32.00        0   0   1   3   4   5   6   5   3   2   1   0   0   0   0   0   0   0   0   0   0   0   0   0   0       32.00
   28.00        0   0   1   3   4   5   6   5   3   2   1   0   0   0   0   0   0   0   0   0   0   0   0   0   0       28.00
   24.00        0   0   1   3   4   5   6   5   3   2   1   0   0   9   9   7   5   4   3   2   2   1   1   1   0       24.00
   20.00        0   0   1   3   4   5   6   5   3   2   1   0   0   0   0   0   0   0   0   0   0   0   0   0   0       20.00
   16.00        0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0       16.00
   12.00        0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0       12.00
    8.00        0   0   0   0   0  10   4   2   1   1   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0        8.00
    4.00        0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0        4.00
    0.0         0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0        0.0
                0.0     8.00    16.00    24.00    32.00    40.00    48.00    56.00    64.00    72.00    80.00    88.00    96.00
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PEM OUTPUT:  SECTION 1 OF 1, SCENARIO  6  PEM EXAMPLE 3   CHEMICAL TRANSFORMATION GAS TO PARTICLE  6-HR AVG CONCENTRATION
STABILITY=F , WIND SPD= 2.50 M/S, WIND DIR=270.00 DEG, MIXING HT=  150.0 M, AVERAGING TIME=  6 HR.
UNCALIBRATED SURFACE DEPOSITION FLUX - MICROGRAMS PER SQUARE METER PER HOUR                     POLLUTANT-2: PARTICLE
            0.0     8.00    16.00    24.00    32.00    40.00    48.00    56.00    64.00    72.00    80.00    88.00    96.00
  96.00     0   0   0   0   0   0   C   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0      96.00
  92.00     C   0   0   0   0   0   C   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0      92.00
  88.00     C   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0      88.00
  84.00     C   0   0   0   0   0   C   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0      84.00
  80.00     0   0   0   0   0   0   C   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0      80.00
  76.00     0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0      76.00
  72.00     0   0   0   0   0   0   C   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0      72.00
  68.00     C   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0      68.00
  64.00     C   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0      64.00
  60.00     0   0   0   0   0   0   C   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0      60.00
  56.00     C   0   0   0   0   0   C   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0      56.00
  52.00     C   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0      52.00
  48.00     0   0 847 475 287 179 114  74  49  32  22  13   8   5   3   2   1   0   0   0   0   0   0   0   0      48.00
  44.00     C   0   0   0   0   0   C   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0      44.00
  40.00     C   0   0   0   0   0   C   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0      40.00
  36.00     C   0  86 185 271 346 415 329 229 144  68   0   0   0   0   0   0   0   0   0   0   0   0   0   0      36.00
  32.00     C   0  86 135 271 346 415 329 229 144  68   0   0   0   0   0   0   0   0   0   0   0   0   0   0      32.00
  28.00     C   0  86 185 271 346 415 329 229 144  68   0   0 627 631 505 387 293 221 167 126  95  62  43  31      28.00
  24.00     C   0  86 185 271 346 415 329 229 144  68   0   0   0   0   0   0   0   0   0   0   0   0   0   0      24.00
  20.00     C   0  86 185 271 346 415 329 229 144  68   0   0   0   0   0   0   0   0   0   0   0   0   0   0      20.00
  16.00     0   0   0   0   0   0   C   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0      16.00
  12.00     C   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0      12.00
   8.00     C   0   0   0   0 734 318 164  91  52  31  18  11   7   4   2   1   1   0   0   0   0   0   0   0       8.00
   4.00     C   0   0   0   0   0   C   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0       4.00
   0.0      C   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0       0.0
            0.0     8.00    16.00    24.00    32.00    40.00    48.00    56.00    64.00    72.00    80.00    88.00    96.00
```

```
                                   POLLUTION EPISODIC MODEL

    OUTPUT:  PEM EXAMPLE 3   CHEMICAL TRANSFORMATION GAS TO PARTICLE  6-HR AVG CONCENTRATION

    HIGHEST PREDICTED CONCENTRATION OF EACH POLLUTANT FOR EACH SCENARIO

    UNCALIBRATED CONCENTRATION IN MICROGRAMS PER CUBIC METER  -  CALIBRATION, POLLUTANT-1:
                                                                  CALIBRATION, POLLUTANT-2:

                                     POLLUTANT-1: GAS                                          POLLUTANT-2: PARTICLE
  SCENARIO  WIND DIRECTION       COORDINATES              CONCENTRATION                  COORDINATES              CONCENTRATION
   NUMBER    SUB-SCENARIO      X(KM)     Y(KM)      UNCALIBRATED    CALIBRATED        X(KM)     Y(KM)      UNCALIBRATED    CALIBRATED

     1            1             8.00     48.00        144.8302         0.0             8.00     48.00        11.7695          0.0
```

```
                              POLLUTION EPISODIC MODEL

     OUTPUT:  PEM EXAMPLE 3   CHEMICAL TRANSFORMATION GAS TO PARTICLE  6-HR AVG CONCENTRATION

     HIGHEST PREDICTED SURFACE DEPOSITION FLUX OF EACH POLLUTANT FOR EACH SCENARIO

     UNCALIBRATED VALUES IN MICROGRAMS PER SQUARE METER PER HOUR  -  CALIBRATION, POLLUTANT-1:
                                                                     CALIBRATION, POLLUTANT-2:

                                   POLLUTANT-1: GAS                                              POLLUTANT-2: PARTICLE
    SCENARIO  WIND DIRECTION       COORDINATES         SURFACE DEPOSITION FLUX             COORDINATES         SURFACE DEPOSITION FLUX
     NUMBER    SUB-SCENARIO      X(KM)     Y(KM)     UNCALIBRATED     CALIBRATED         X(KM)     Y(KM)     UNCALIBRATED     CALIBRATED

       1            1             8.00      48.00      5213.8828          0.0               8.00      48.00       847.4036          0.0
    IHC002I STOP    0
```

APPENDIX F

PEM FORTRAN LISTING

The PEM (Version 82360) computer program was developed and tested on the IBM computers at the Oak Ridge National Laboratory. The program was later modified slightly to run it on the UNIVAC computer at Research Triangle Park. A listing of this UNIVAC-compatible FORTRAN program follows. This listing clearly shows the modifications made to adapt the PEM computer code from the IBM to the UNIVAC. A summary of the statements (identified by their line numbers in the listing) required for each computer is given below:

IBM	UNIVAC
208	209
-	1524
-	1577
-	1639
4362	4359-4361
4389	4386-4388
4415	4412-4414

```
RAPS*PEM(1).PROGRAM(4)
C                                                                       00000010
C                                                                       00000020
C                                                                       00000030
C                  *** PEM   (VERSION  82360) ***                       00000040
C                                                                       00000050
C                                                                       00000060
C                        POLLUTION EPISODIC MODEL                       00000070
C                               INCLUDING                               00000080
C      DEPOSITION, SEDIMENTATION, AND CHEMICAL TRANSFORMATION           00000090
C                             OF POLLUTANTS                             00000100
C                                                                       00000110
C                                                                       00000120
C *** PEM PROGRAM DEVELOPMENT : --- DECEMBER 1982                       00000130
C                                                                       00000140
C     K. SHANKAR RAO AND MARTHA M. STEVENS                              00000150
C     ATMOSPHERIC TURBULENCE AND DIFFUSION LABORATORY (ATDL)            00000160
C     NATIONAL OCEANIC AND ATMOSPHERIC ADMINISTRATION (NOAA)            00000170
C     U.S. DEPARTMENT OF COMMERCE                                       00000180
C     P.O. BOX - E                                                      00000190
C     OAK RIDGE, TENN 37830                                             00000200
C                                                                       00000210
C     PHONE: (615) 576-1238  OR  1241                                   00000220
C             FTS: 626-1238  OR  1241                                   00000230
C                                                                       00000240
C     ( THIS WORK WAS DONE UNDER AN INTERAGENCY AGREEMENT                00000250
C     BETWEEN THE ENVIRONMENTAL PROTECTION AGENCY AND THE               00000260
C     NATIONAL OCEANIC AND ATMOSPHERIC ADMINISTRATION )                 00000270
C                                                                       00000280
C                                                                       00000290
C *** EXTENDED ABSTRACT : PEM (VERSION 82360).                          00000300
C                                                                       00000310
C        PEM IS AN URBAN SCALE (UPTO 60 KM DISTANCES) AIR QUALITY       00000320
C     DISPERSION-DEPOSITION MODEL CAPABLE OF PREDICTING SHORT-TERM      00000330
C     (1 TO 24-HOUR) AVERAGE SURFACE CONCENTRATIONS AND DEPOSITION      00000340
C     FLUXES OF ONE OR TWO GASEOUS OR PARTICULATE POLLUTANTS AT         00000350
C     UP TO A MAXIMUM OF 50X50 GROUND-LEVEL RECEPTORS.  PREDICTIONS ARE 00000360
C     BASED ON STEADY-STATE GAUSSIAN PLUME HYPOTHESIS, BRIGGS' PLUME    00000370
C     RISE FORMULATIONS, AND PASQUILL-GIFFORD (PG) STABILITY CLASS-     00000380
C     IFICATION AND DISPERSION PARAMETER CURVES.  UP TO 300 INDIVIDUAL  00000390
C     POINT SOURCES AND UP TO 50 AREA SOURCES MAY BE INCLUDED IN THE    00000400
C     INPUTS TO THE MODEL.  CALCULATIONS ARE PERFORMED FOR EACH HOUR    00000410
C     USING THE SPECIFIED HOURLY METEOROLOGICAL DATA. UP TO 24 DIFFERENT00000420
C     SETS OF HOURLY METEOROLOGICAL DATA MAY BE SPECIFIED AS INPUT FOR  00000430
C     THE DETERMINATION OF AIR QUALITY FOR 24 DISTINCT WEATHER          00000440
C     SCENARIOS.  POLLUTANT CONCENTRATIONS AND DEPOSITION FLUXES FOR A  00000450
C     2 TO 24 AVERAGING PERIOD ARE CALCULATED BY AVERAGING THE CORRES-  00000460
C     PONDING VALUES CALCULATED FOR EACH HOUR IN THE PERIOD.            00000470
C                                                                       00000480
C        PEM IS BASED ON THE TEXAS EPISODIC MODEL (TEM, VERSION 8)      00000490
C     DEVELOPED BY THE TEXAS AIR CONTROL BOARD (1979).  TEM USES THE    00000500
C     GAUSSIAN PLUME CONCENTRATION ALGORITHMS DEVELOPED FOR NON-REACTIVE00000510
C     POLLUTANTS AND A PERFECTLY REFLECTING LOWER BOUNDARY.  CHEMICAL   00000520
C     AND PHYSICAL DEPLETION PROCESSES ARE THEREFORE IGNORED, EXCEPT FOR00000530
C     AN OPTION WHICH ALLOWS A SIMPLE EXPONENTIAL DECAY OF POLLUTANT    00000540
C     WITH TRAVEL TIME.  THIS METHOD REQUIRES AN ACCURATE ESTIMATE OF   00000550
C     THE POLLUTANT'S HALF-LIFE.                                        00000560
C                                                                       00000570
C        IN CONTRAST, PEM EXPLICITLY ACCOUNTS FOR THE DRY DEPOSITION,   00000580
C     GRAVITATIONAL SETTLING, AND A FIRST-ORDER CHEMICAL TRANSFORMATION 00000590
C     OR DECAY OF GASEOUS OR PARTICULATE POLLUTANTS (OF ANY SIZE) IN    00000600
C     THE CONCENTRATION ALGORITHMS.  THESE ALGORITHMS, BASED ON EXACT   00000610
C     SOLUTIONS OF A GRADIENT-TRANSFER ('K-THEORY') MODEL, WERE GIVEN BY00000620
C     RAO (1981, 1982) AS ANALYTICAL EXTENSIONS OF THE WIDELY-USED      00000630
C     GAUSSIAN PLUME DISPERSION ALGORITHMS UNDER VARIOUS ATMOSPHERIC    00000640
C     STABILITY AND MIXING CONDITIONS.  THUS, PEM TREATS DEPOSITION,    00000650
C     SEDIMENTATION, AND CHEMICAL TRANSFORMATION IN A PHYSICALLY REAL-  00000660
C     ISTIC AND STRAIGHTFORWARD MANNER, AND IT IS SUBJECT TO THE SAME   00000670
C     BASIC ASSUMPTIONS AND LIMITATIONS ASSOCIATED WITH ALL GAUSSIAN-   00000680
C     PLUME TYPE MODELS.  FOR FURTHER DETAILS REGARDING THE GRADIENT-   00000690
C     TRANSFER MODEL FORMULATIONS, ANALYTICAL SOLUTIONS, PARAMETERI-    00000700
C     ZATIONS, AND THE DEVELOPMENT OF THE ALGORITHMS FOR PEM, THE USER  00000710
C     SHOULD CONSULT THE REPORTS BY RAO (1981, 1982).                   00000720
C                                                                       00000730
C       BASED ON THE NUMBER OF POLLUTANTS (NPOL=1 OR 2) AND THE CHEMI-  00000740
C     CAL TRANSFORMATION/DECAY OPTION PARAMETER (ICT=0 OR 1) SPECIFIED  00000750
C     IN THE INPUT TO THE MODEL, PEM PROGRAM DOES ONE OF THE FOLLOWING: 00000760
```

```
C                                                                       00000770
C     (1) IF NPOL=1 AND ICT=0 OR 1, SURFACE CONCENTRATIONS AND DEPOSI-  00000780
C        TION FLUXES OF ONE GASEOUS OR PARTICULATE POLLUTANT, WITH THE  00000790
C        GIVEN DEPOSITION AND SETTLING VELOCITIES, VD1 AND W1 RESPECTI- 00000800
C        VELY, ARE CALCULATED.  IF ICT=1, THEN CHEMICAL DECAY OF POLLU- 00000810
C        TANT IS ALSO CONSIDERED IF THE DECAY RATE XKT > 0. IS GIVEN    00000820
C        IN PERCENT PER HOUR.                                           00000830
C                                                                       00000840
C     (2) IF NPOL=2 AND ICT=0, SURFACE CONCENTRATIONS AND DEPOSITION    00000850
C        FLUXES OF TWO DIFFERENT AND UNCOUPLED GASEOUS OR PARTICULATE   00000860
C        POLLUTANT SPECIES WITH THE GIVEN DEPOSITION AND SETTLING VELOC-00000870
C        ITIES VD1 AND W1 (FOR SPECIES-1) AND VD2 AND W2 (FOR SPECIES-2)00000880
C        RESPECTIVELY, ARE CALCULATED.  EMISSION RATES FOR BOTH SPECIES 00000890
C        MAY BE DIFFERENT.  CHEMICAL DECAY IS NOT CONSIDERED FOR EITHER 00000900
C        SPECIES EVEN IF A VALUE OF XKT > 0. IS SPECIFIED.              00000910
C                                                                       00000920
C     (3) IF NPOL=2 AND ICT=1, THE TWO GASEOUS OR PARTICULATE POLLUTANT 00000930
C        SPECIES ARE COUPLED THROUGH A FIRST-ORDER CHEMICAL TRANSFORMA- 00000940
C        TION.  THE SURFACE CONCENTRATIONS AND DEPOSITION FLUXES OF BOTH00000950
C        THE PRIMARY POLLUTANT (SPECIES-1 OR REACTANT) AS WELL AS THE   00000960
C        SECONDARY POLLUTANT (SPECIES-2 OR REACTION PRODUCT) ARE CALCU- 00000970
C        LATED.  THE CHEMICAL TRANSFORMATION RATE (XKT > 0.) SHOULD BE  00000980
C        GIVEN.  BOTH SPECIES MAY BE GIVEN NON-EQUAL DEPOSITION AND SET-00000990
C        TLING VELOCITIES.  A NON-ZERO DIRECT EMISSION RATE FOR THE     00001000
C        SECONDARY POLLUTANT FROM  THE POINT AND/OR AREA SOURCES MAY    00001010
C        ALSO BE SPECIFIED AS INPUT FOR THIS CASE.                      00001020
C                                                                       00001030
C        FOR FURTHER DETAILS REGARDING THE USE OF THE PEM AND ITS I/O   00001040
C     OPTIONS, INPUT PARAMETERS AND UNITS, AND EXAMPLE PROBLEMS, THE    00001050
C     USER SHOULD CONSULT THE PEM USER'S GUIDE BY RAO AND STEVENS (1982)00001060
C                                                                       00001070
C                            *** REFERENCES ***                         00001080
C                                                                       00001090
C     (1) STAFF OF THE TEXAS AIR CONTROL BOARD, 1979: USER'S GUIDE :    00001100
C         TEXAS EPISODIC MODEL.  TEXAS AIR CONTROL BOARD, PERMITS       00001110
C         SECTION, AUSTIN, TEXAS 78723, 215 PP.                         00001120
C                                                                       00001130
C     (2) RAO, K. S., 1981: ANALYTICAL SOLUTIONS OF A GRADIENT-TRANSFER 00001140
C         MODEL FOR PLUME DEPOSITION AND SEDIMENTATION.  EPA-          ,00001150
C         U.S.E.P.A., RESEARCH TRIANGLE PARK, NC;                       00001160
C         NOAA TECH. MEMO. ERL/ARL-109, NOAA-ATDL, OAK RIDGE, TN 37830, 00001170
C         75 PP.  ATDL CONTRIBUTION FILE NO. 81/14.                     00001180
C                                                                       00001190
C     (3) RAO, K. S., 1982: GAUSSIAN PLUME CONCENTRATION ALGORITHMS WITH00001200
C         DEPOSITION, SEDIMENTATION, AND CHEMICAL TRANSFORMATION.       00001210
C         EPA-          , RESEARCH TRIANGLE PARK, NC;                   00001220
C         NOAA TECH. MEMO. ERL/ARL-   , NOAA-ATDL, OAK RIDGE, TN 37830. 00001230
C         ATDL CONTRIBUTION FILE NO. 82/27.                             00001240
C                                                                       00001250
C     (4) RAO, K. S., AND M. M. STEVENS, 1982:  POLLUTION EPISODIC      00001260
C         MODEL:  USER'S GUIDE.  EPA-               , RESEARCH          00001270
C         TRIANGLE PARK, NC.                                            00001280
C         NOAA TECH. MEMO. ERL/ARL-   , NOAA-ATDL, OAK RIDGE, TN 37830. 00001290
C         ATDL CONTRIBUTION FILE NO. 82/28.                             00001300
C                                                                       00001310
C                                                                       00001320
C                                                                       00001330
C *** PEM (VERSION 82360) : FORTRAN LISTING.                            00001340
C                                                                       00001350
C                                                                       00001360
C                                                                       00001370
C                                                                       00001380
C                                                                       00001390
C *** COMMON BLOCKS, DIMENSIONS, AND DATA STATEMENTS.                   00001400
C                                                                       00001410
C                                                                       00001420
      COMMON/PEMCOM/CONC(50,50,2),SDF(50,50,2),  TT(20),                00001430
     1 XP(300),YP(300),EP(300,2),HP(300),DP(300),VP(300),TP(300),       00001440
     2 XA(50),YA(50),EA(50,2),SIZE(50),                                 00001450
     3 WD(24),WS(24),TA(24),HMIX(24),PEN(24),                           00001460
     4 AX(7,3),BX(7,3),P(7),SCLAB(7),DTDZ(2),  SECTAN(16),              00001470
     5 XSWC,YSWC,GRID,LX,LY,      A(2),B(2),POLNAM(3,2),CALNAM(7,2),    00001480
     6 ITA,IRD,IWR,IDSK,          D80,D47,D8047,DIST,DELTA,             00001490
     7 ESH(2),PEAK,IBUOY,IRISE,IDWN,EFF,XS,    UINV,WVEC,               00001500
     8 NAS,NPS,INDEX,IGRID,IAV,ISCEN,IWDOPT,IWD,ISC,IPS,                00001510
     9 NTOPT,NWDOPT,NWSOPT,NSCEN,NLIST,NARRAY,NTAPE,NCSOPT,NMAX,        00001520
     * NSTDWN,INTER,NPRINT                                              00001530
```

```
C
      COMMON/PARM1/NPOL,ICT,VD1,W1,VD2,W2,TAUC                          00001540
      COMMON/PARM1A/GAMMA                                               00001550
      COMMON/PARM2/ISPEC,UTAUC,Q2Q1,XCT,EXCT                            00001560
      COMMON/PARM2A/AA,BA                                               00001570
      COMMON/PARM3/HC,VDC1,WC1,VDC2,WC2                                 00001580
      COMMON/PARM4/V11,V21,V12,V22,V13                                  00001590
      COMMON/PARM5/D11,D21,D12,D22,D31,D32,D33,D6                       00001600
      COMMON/PARM6/R11,R21,R12,R22,R13,R23,R31,R41,R32,R42              00001610
      COMMON/PARM7/QZC1,QZC2                                            00001620
      COMMON/BLOCK1/PI,SQPI,SQRT2,A1B,A1C                               00001630
      COMMON/BLOCK2/AI,BI,EPSABS,EPSREL,LW,NIW                          00001640
      COMMON/EXPCHK/EXPMAX,EXPMIN,ETAMAX                                00001650
C                                                                       00001660
      EXTERNAL FUN3                                                     00001670
      REAL*8 FUN3                                                       00001680
      REAL*8 WORK(800),AI,BI,EPSABS,EPSREL,RESULT,ABSERR,T1A,T2A        00001690
      DIMENSION IW(102)                                                 00001700
      DIMENSION PRL(2,2),DWL(4),ANGLIM(7)                               00001710
      DIMENSION ITABLE(5,10),EPSLIM(10)                                 00001720
      DIMENSION AAR(6),BAR(6),CX1(7),DX1(7),CX2(7),DX2(7)               00001730
      DIMENSION XA1(5),XA2(5),XA2C(5),RCA1(5),RCA2(5)                   00001740
      DIMENSION RCA2CT(5,50),QA2QA1(50),TERMB2(5)                       00001750
C                                                                       00001760
      DATA PRL/4HMOME,4HNTUM,4HBUOY,4HANCY/                             00001770
      DATA DWL/4H    ,4H    ,4HDOWN,4HWASH/                             00001780
      DATA EPSLIM/.12427,.16511,.24504,.35884,.46373,                   00001790
     1            .55868,.64350,.69482,.71890,.78540/                   00001800
      DATA ITABLE/0,0,0,0,0, 0,0,0,0,1, 0,0,0,1,1, 0,0,1,1,1, 0,0,1,1,2,00001810
     1            0,1,1,2,2, 0,1,1,2,3, 0,1,2,2,3, 0,1,2,3,3, 0,1,2,3,4/00001820
      DATA ANGLIM/0.610865,0.488692,0.366519,0.244346,                  00001830
     1 0.244346,0.183260,0.122173/                                      00001840
      DATA CX1/.495,.310,.197,.122,.122,.0934,.0625/                    00001850
      DATA DX1/.873,.897,.908,.916,.916,.912,.911/                      00001860
      DATA CX2/.606,.523,.285,.193,.193,.141,.080/                      00001870
      DATA DX2/.851,.840,.867,.865,.865,.868,.884/                      00001880
      DATA AAR/.4,.4,.33,.22,.15,.06/                                   00001890
      DATA BAR/.91,.91,.86,.80,.75,.71/                                 00001900
C                                                                       00001910
C                                                                       00001920
C                                                                       00001930
C *** DEFINE PROGRAM CONSTANTS.                                         00001940
C                                                                       00001950
      PI=3.14159                                                        00001960
      SQPI=SQRT(PI)                                                     00001970
      SQRT2=SQRT(2.)                                                    00001980
      A1B=1000./(SQRT2*SQPI)                                            00001990
      A1C=2.*SQPI                                                       00002000
      AI=0.                                                             00002010
      BI=1.                                                             00002020
      EPSABS=1.0E-4                                                     00002030
      EPSREL=1.0E-4                                                     00002040
      LW=800                                                            00002050
      NIW=102                                                           00002060
C     EXPMAX=174.                                                       00002070
      EXPMAX= 87.                                                       00002080
      EXPMIN=50.
      ETAMAX=SQRT(EXPMAX)                                               00002090
C                                                                       00002100
      WRITE (IWR,5432)                                                  00002110
 5432 FORMAT ('1',///////46X,'PEM   (VERSION  82360)'/////              00002120
     1 45X,'POLLUTION EPISODIC MODEL'/////                              00002130
     2 52X,'INCLUDING'//                                                00002140
     3 30X,'DEPOSITION, SEDIMENTATION, AND CHEMICAL TRANSFORMATION'//   00002150
     4 50X,'OF POLLUTANTS'/)                                            00002160
C                                                                       00002170
      INDEX=0                                                           00002180
C                                                                       00002190
C  CALL INPUT MODULE TO READ ALL WEATHER AND SOURCE INFORMATION,        00002200
C     DEPOSITION AND SEDIMENTATION VELOCITIES OF POLLUTANT SPECIES,     00002210
C     AND CHEMICAL DECAY OR TRANFORMATION RATE.                         00002220
C                                                                       00002230
C     ************                                                      00002240
      CALL INMOD                                                        00002250
C     ************                                                      00002260
C                                                                       00002270
      VD136=VD1*36.                                                     00002280
                                                                        00002290
      VD236=VD2*36.
C
C
C *** DETERMINE VALUE OF PARAMETER ISPEC.
C     ISPEC IS AN INTERNAL ROUTING PARAMETER USED IN PEM
C     TO DETERMINE THE APPROPRIATE CONCENTRATION ALGORITHMS
C     TO BE USED FOR A GIVEN PROBLEM.
C     VALUE OF ISPEC  IS BASED ON NUMBER OF POLLUTANTS,
C     AND CHEMICAL TRANSFORMATION OPTION PARAMETER.
      IF(NPOL.EQ.2) GO TO 41
C     ONLY ONE POLLUTANT SPECIES.  CHEMICAL DECAY CAN BE CONSIDERED
C     BY SETTING ICT = 1 AND XKT > 0.
      ISPEC=1
      GO TO 43
C
C     TWO POLLUTANT SPECIES.
   41 IF(ICT.EQ.1) GO TO 42
C     NO CHEMICAL COUPLING. THE TWO SPECIES ARE INDEPENDENT
C     OF EACH OTHER.  CHEMICAL DECAY IS NOT CONSIDERED FOR
C     EITHER SPECIES.
      ISPEC=2
      GO TO 43
C
C     CHEMICAL COUPLING EXISTS BETWEEN SPECIES-1 (REACTANT)
C     AND SPECIES-2 (PRODUCT).
   42 ISPEC=3
   43 CONTINUE
C
C
C
C *** DEFINE TIME-AVERAGING MULTIPLIER CONSTANTS.
C
      IF(NTOPT.EQ.1) STCONV = 1.
      IF(NTOPT.EQ.2) STCONV= 0.04166667
      IF(NTOPT.EQ.3) STCONV= 1.0/FLOAT(NSCEN)
C
      INDEX=1
C
C  CALL INPUT MODULE TO BRING IN WEATHER DATA FOR ONE SCENARIO
C    (NUMBER OF SCENARIO = ISCEN).
C
C     ************
100   CALL INMOD
C     ************
C
C  CALCULATE WIND VECTOR (WVEC) FOR SCENARIO. IFLAG IS USED BELOW
C    (STMT. 275) TO DETERMINE METHOD OF RESTRICTING THE AREA OF THE
C    RECEPTOR GRID AFFECTED BY EACH SOURCE.
C
175   IF(NWDOPT.EQ.1) GO TO 200
      DO 180 IWD=1,16
      DETA=ABS(WD(ISCEN)-SECTAN(IWD))
      IF(DETA.LE.0.19634954) GO TO 185
180   CONTINUE
185   GO TO 205
200   WD(ISCEN)=SECTAN(IWD)
205   IF(IWD.LT.8.OR.IWD.GT.10) GO TO 210
      IFLAG=1
      GO TO 241
210   IF(IWD.NE.11) GO TO 215
      IFLAG=2
      GO TO 241
215   IF(IWD.LT.12.OR.IWD.GT.14) GO TO 220
      IFLAG=3
      GO TO 241
220   IF(IWD.NE.15) GO TO 225
      IFLAG=4
      GO TO 241
225   IF(IWD.LT.16.AND.IWD.GT.2) GO TO 230
      IFLAG=5
      GO TO 241
230   IF(IWD.NE.3) GO TO 235
      IFLAG=6
      GO TO 241
235   IF(IWD.LT.4.OR.IWD.GT.6) GO TO 240
      IFLAG=7
      GO TO 241                                                         00003070
  240 IFLAG=8                                                           00003080
  241 WVEC= WD(ISCEN) + 3.14159265                                      00003090
      IF(WVEC.GT.6.2831853) WVEC=WVEC - 6.2831853                       00003100
      WDV=4.712388981-WD(ISCEN)                                         00003110
      IF(WDV.LT.0.)WDV=WDV+6.283185307                                  00003120
      WDPANG=WDV+ANGLIM(ISC)                                            00003130
      WDMANG=WDV-ANGLIM(ISC)                                            00003140
C                                                                       00003150
C  CALL AUTGRD TO CALCULATE RECEPTOR GRID PARAMETERS AUTOMATICALLY.     00003160
C     ************                                                      00003170
      IF(IGRID.EQ.1) CALL AUTGRD                                        00003180
C     ************                                                      00003190
C                                                                       00003200
C                                                                       00003210
C *** INITIALIZATION.                                                   00003220
C                                                                       00003230
C  INITIALIZE CONCENTRATION AND SURFACE DEPOSITION FLUX ARRAYS          00003240
      IF(NTOPT.GT.1.AND.ISCEN.GT.1) GO TO 4                             00003250
      DO 2 I=1,LX                                                       00003260
      DO 2 J=1,LY                                                       00003270
      CONC(I,J,1)=0.                                                    00003280
      SDF(I,J,1)=0.                                                     00003290
      IF(ISPEC.EQ.1.AND.NCSOPT.EQ.0) GO TO 2                            00003300
      CONC(I,J,2)=0.                                                    00003310
      SDF(I,J,2)=0.                                                     00003320
    2 CONTINUE                                                          00003330
C                                                                       00003340
C                                                                       00003350
C                                                                       00003360
    4 VGRID= 1./GRID                                                    00003370
      GRIDSQ= GRID*GRID                                                 00003380
      ELX= LX                                                           00003390
      ELY= LY                                                           00003400
      XB1= XSWC + 0.5*GRID                                              00003410
      XB2= XSWC + (ELX-0.5)*GRID                                        00003420
      YB1= YSWC + 0.5*GRID                                              00003430
      YB2= YSWC + (ELY-0.5)*GRID                                        00003440
C                                                                       00003450
C  IF NO AREA SOURCES, SKIP AREA SOURCE CALCULATIONS.                   00003460
      IF(NAS.LT.1) GO TO 245                                            00003470
C                                                                       00003480
C                                                                       00003490
C                                                                       00003500
C***  A R E A   S O U R C E   C A L C U L A T I O N S  ***              00003510
C                                                                       00003520
C    IWV HELPS DETERMINE THE PATTERN OF GRID SQUARES AFFECTED BY EACH   00003530
C    AREA SOURCE.  PATTERN DEPENDS ONLY ON WIND DIRECTION.              00003540
C    EPS IS THE ANGLE BETWEEN THE WIND VECTOR AND THE NEAREST           00003550
C    COORDINATE AXIS.                                                   00003560
C                                                                       00003570
      IWV= 1 + WVEC/0.78540                                             00003580
      GO TO (2411,2412,2413,2414,2415,2416,2417,2418),IWV               00003590
 2411 ITABX=1                                                           00003600
      ISIGNX=1                                                          00003610
      ISIGNY=1                                                          00003620
      EPS= WVEC                                                         00003630
      GO TO 2419                                                        00003640
 2412 ITABX=0                                                           00003650
      ISIGNX=1                                                          00003660
      ISIGNY=1                                                          00003670
      EPS= 1.5708 - WVEC                                                00003680
      GO TO 2419                                                        00003690
 2413 ITABX=0                                                           00003700
      ISIGNX=1                                                          00003710
      ISIGNY=-1                                                         00003720
      EPS= WVEC - 1.57080                                               00003730
      GO TO 2419                                                        00003740
 2414 ITABX=1                                                           00003750
      ISIGNX=1                                                          00003760
      ISIGNY=-1                                                         00003770
      EPS= 3.1416 - WVEC                                                00003780
      GO TO 2419                                                        00003790
 2415 ITABX=1                                                           00003800
      ISIGNX=-1                                                         00003810
      ISIGNY=-1                                                         00003820
      EPS= WVEC - 3.1416                                                00003830
      GO TO 2419                                                        00003830
 2416 ITABX=0                                                           00003840
      ISIGNX=-1                                                         00003850
      ISIGNY=-1                                                         00003860
      EPS= 4.7124 - WVEC                                                00003870
      GO TO 2419                                                        00003880
 2417 ITABX=0                                                           00003890
      ISIGNX=-1                                                         00003900
      ISIGNY=1                                                          00003910
      EPS= WVEC - 4.7124                                                00003920
      GO TO 2419                                                        00003930
 2418 ITABX=1                                                           00003940
      ISIGNX=-1                                                         00003950
      ISIGNY=1                                                          00003960
      EPS= 6.2832 - WVEC                                                00003970
 2419 IF(ITABX.EQ.0) GO TO 2420                                         00003980
      ITABY=0                                                           00003990
      INCRX=0                                                           00004000
      INCRY=1                                                           00004010
      GO TO 2421                                                        00004020
 2420 ITABY=1                                                           00004030
      INCRX=1                                                           00004040
      INCRY=0                                                           00004050
 2421 DO 2422 L=1,10                                                    00004060
      IF(EPS.GT.EPSLIM(L)) GO TO 2422                                   00004070
      IEPS=L                                                            00004080
      GO TO 2423                                                        00004090
 2422 CONTINUE                                                          00004100
      IEPS=10                                                           00004110
C                                                                       00004120
C     REDUCE STABILITY CLASS BY 1 (EXCEPT FOR ISC=1) TO SIMULATE        00004130
C     SURFACE TURBULENCE IN URBAN CONDITIONS.                           00004140
C                                                                       00004150
 2423 IA= ISC-1                                                         00004160
      IF(IA.EQ.0) IA=1                                                  00004170
      AA= AAR(IA)                                                       00004180
      BA= BAR(IA)                                                       00004190
      BA1=2.*(1.-BA)                                                    00004200
      DXA=1000.*GRID/COS(EPS)                                           00004210
      UPL=WS(ISCEN)                                                     00004220
      UINV=1./UPL                                                       00004230
      UINV1=UINV/100.                                                   00004240
C                                                                       00004250
C     DEFINE NONDIMENSIONAL DEPOSITION AND SEDIMENTATION PARAMETERS.    00004260
C                                                                       00004270
C     ISPEC = 1 OR 2 OR 3                                               00004280
      BAVD1=0.01*VD1*BA1                                                00004290
      VDC1=VD1*UINV1                                                    00004300
      WC1=W1*UINV1                                                      00004310
      V11=VDC1-0.5*WC1                                                  00004320
      V21=VDC1-WC1                                                      00004330
      IF(V21.EQ.0.) GO TO 44                                            00004340
      R11=V11/V21                                                       00004350
      R21=0.5*WC1/V21                                                   00004360
   44 IF(ISPEC.EQ.1) GO TO 46                                           00004370
C                                                                       00004380
C     ISPEC = 2 OR 3                                                    00004390
      BAVD2=0.01*VD2*BA1                                                00004400
      VDC2=VD2*UINV1                                                    00004410
      WC2=W2*UINV1                                                      00004420
      V12=VDC2-0.5*WC2                                                  00004430
      V22=VDC2-WC2                                                      00004440
      IF(V22.EQ.0.) GO TO 45                                            00004450
      R12=V12/V22                                                       00004460
      R22=0.5*WC2/V22                                                   00004470
   45 IF(ISPEC.EQ.2) GO TO 47                                           00004480
C                                                                       00004490
C     ISPEC = 3                                                         00004500
      V13=V11-0.5*(WC1-WC2)                                             00004510
      IF(V21.EQ.0.) GO TO 46                                            00004520
      R13=V13/V21                                                       00004530
      R23=0.5*WC2/V21                                                   00004540
C                                                                       00004550
C     ISPEC = 1 OR 3                                                    00004560
   46 UTAUC=TAUC*UPL                                                    00004570
   47 CONTINUE                                                          00004580
C                                                                       00004590
C                                                                       00004600
```

```
C     CALCULATE RELATIVE CONCENTRATIONS AT A RECEPTOR LOCATED AT THE
C     CENTER OF THE CALCULATION GRID SQUARE CONTAINING THE AREA SOURCE
C     EMISSIONS, AND AT THE CENTER OF EACH OF THE FOUR GRID SQUARES
C     IMMEDIATELY DOWNWIND OF THE SOURCE.
C
C     FIRST DEFINE DOWNWIND DISTANCES TO THE LEADING AND TRAILING EDGES,
C     AND MID-POINTS OF THE FIVE CALCULATION GRID SQUARES.
      XA1(1)=0.0
      XA2(1)=0.5*DXA
C
      DO 102 I=1,5
      SZ2=AA*(XA2(I)**BA)
      IF(SZ2.GT.5000.) SZ2=5000.
      XA2C(I)=XA2(I)/(SQRT2*SZ2)
C
      IF(I.EQ.5) GO TO 102
      XA1(I+1)=XA2(I)
      XA2(I+1)=XA1(I+1)+DXA
  102 CONTINUE
C
      K=1
      IF(ISPEC.NE.3) GO TO 104
C
C     START LOOP ON ALL AREA SOURCES IF ISPEC = 3
      DO 114 K=1,NAS
      IF(EA(K,1).EQ.0.) EA(K,1)=1.E-6
      QA2QA1(K)=EA(K,2)/EA(K,1)
      IF(K.EQ.1) GO TO 103
      IF(QA2QA1(K).EQ.QA2QA1(K-1)) GO TO 112
  103 Q2Q1=QA2QA1(K)
      G42PX1=Q2Q1
C
  104 G41PX1=1.
      IF(ISPEC.EQ.2) G42PX1=1.
C
C     START LOOP ON FIVE CALCULATION GRID SQUARES WITH RECEPTORS.
      DO 111 I=1,5
      X1A=XA1(I)
      X2A=XA2(I)
      X2CA=XA2C(I)
C
C     ISPEC = 1 OR 2 OR 3
      D31=2.*V11*X2CA
      D11=WC1*X2CA
      D21=D11*D11
      R31=1.+2.*D21
      R41=2.*D11/SQPI
      IF(ISPEC.EQ.1) GO TO 107
C
C     ISPEC = 2 OR 3
      D32=2.*V12*X2CA
      D12=WC2*X2CA
      D22=D12*D12
      R32=1.+2.*D22
      R42=2.*D12/SQPI
      IF(ISPEC.EQ.2) GO TO 107
C
C     ISPEC = 3
      D33=2.*V13*X2CA
      D6=4.*SQPI*(V21-V22)*X2CA
C
  107 IF(ICT.EQ.0) XCT=0.
      IF(ICT.EQ.1) XCT=X2A/UTAUC
      EXCT=EXP(-XCT)
      IF(ISPEC.EQ.3) GO TO 108
C
C     ISPEC = 1 OR 2
C     ************
      CALL PSG4P(G41PX2,G42PX2)
C     ************
      IF(ICT.EQ.1) GO TO 108
C     ISPEC = 1 WITH ICT = 0 OR ISPEC = 2
      RCA1(I)=(G41PX1-G41PX2)/BAVD1
      IF(RCA1(I).LT.0.) RCA1(I)=0.0
      G41PX1=G41PX2
      IF(ISPEC.EQ.1) GO TO 111
C     ISPEC = 2
```

```
      RCA2(I)=(G42PX1-G42PX2)/BAVD2
      IF(RCA2(I).LT.0.) RCA2(I)=0.0
      G42PX1=G42PX2
      GO TO 111
C
C     ISPEC = 1 WITH ICT = 1 OR ISPEC = 3
  108 IF(K.GT.1) GO TO 109
      T1A=X1A/UTAUC
      T2A=X2A/UTAUC
C     COMPUTE INTEGRAL FUNC=F3(T1A,T2A); FUN3 IS THE INTEGRAND FUNCTION.
C     ************
      CALL D01AJF(FUN3,T1A,T2A,EPSABS,EPSREL,RESULT,
     1   ABSERR,WORK,LW,IW,NIW,IFAIL)
C     ************
      FUNC=RESULT
      TERMB1=FUNC
      IF(ISPEC.EQ.1) GO TO 106
      TERMB2(I)=GAMMA*FUNC*VDC1/VDC2
      IF(ISPEC.EQ.3) GO TO 109
C
C     ISPEC = 1 WITH ICT = 1
  106 RCA1(I)=((G41PX1-G41PX2)/VDC1-TERMB1)/BA1
      IF(RCA1(I).LT.0.) RCA1(I)=0.0
      RCA1(I)=RCA1(I)*UINV
      G41PX1=G41PX2
      GO TO 111
C
C     ISPEC = 3
C     ************
  109 CALL PSG4P(G41PX2,G42PX2)
C     ************
      IF(K.GT.1) GO TO 110
      TERMA1=(G41PX1-G41PX2)/VDC1
      DUM1=(TERMA1-TERMB1)/BA1
      IF(DUM1.LT.0.) DUM1=0.0
      RCA1(I)=DUM1*UINV
      G41PX1=G41PX2
  110 TERMA2=(G42PX1-G42PX2)/VDC2
      DUM2=(TERMA2+TERMB2(I))/BA1
      IF(DUM2.LT.0.) DUM2=0.0
      RCA2CT(I,K)=DUM2*UINV
      G42PX1=G42PX2
C
  111 CONTINUE
C     END LOOP ON I=1,5 CALCULATION GRID SQUARES.
      GO TO 114
C
  112 DO 113 I=1,5
      RCA2CT(I,K)=RCA2CT(I,K-1)
  113 CONTINUE
C
  114 CONTINUE
C     END LOOP ON K=1,NAS AREA SOURCES IF ISPEC = 3
C
C
C LOOP THROUGH ALL AREA SOURCES.  EMISSIONS FROM EACH AREA SOURCE
C   ARE APPORTIONED AMONG THE RECEPTOR GRID SQUARES WHOLLY OR
C   PARTIALLY COVERED BY THE SOURCE.  EACH AFFECTED RECEPTOR GRID
C   SQUARE IS TREATED AS A SOURCE.
C
C     START LOOP ON K=1,NAS AREA SOURCES.
      DO 2429 K=1,NAS
      AREA= SIZE(K)*SIZE(K)
      AX1= XA(K)
      AX2= AX1 + SIZE(K)
      NX1= (AX1-XSWC)*VGRID + 5.
      NX2= (AX2-XSWC)*VGRID + 5.
      IF(NX1.GT.LX+8.OR.NX2.LT.1) GO TO 2429
      IF(NX1.GE.1) GO TO 32
      NX1= 1
      AX1= XSWC - 4.*GRID
 32   IF(NX2.LE.LX+8) GO TO 34
      NX2= LX+8
      AX2= XSWC + (ELX + 4.)*GRID
 34   X1= XSWC + (FLOAT(NX1)-5.)*GRID
      X2= XSWC + (FLOAT(NX2)-4.)*GRID
      AY1= YA(K)
      AY2= AY1 + SIZE(K)                                                00006150
      NY1= (AY1-YSWC)*VGRID + 5.                                        00006160
      NY2= (AY2-YSWC)*VGRID + 5.                                        00006170
      IF(NY1.GT.LY+8.OR.NY2.LT.1) GO TO 2429                            00006180
      IF(NY1.GE.1) GO TO 36                                             00006190
      NY1= 1                                                            00006200
      AY1= YSWC - 4.*GRID                                               00006210
 36   IF(NY2.LE.LY+8) GO TO 38                                          00006220
      NY2= LY+8                                                         00006230
      AY2= YSWC + (ELY + 4.)*GRID                                       00006240
 38   Y1= YSWC + (FLOAT(NY1)-5.)*GRID                                   00006250
      Y2= YSWC + (FLOAT(NY2)-4.)*GRID                                   00006260
C                                                                       00006270
C     START LOOP ON IX=NX1,NX2 COLUMNS OF THE RECEPTOR GRID.            00006280
      DO 2428 IX=NX1,NX2                                                00006290
      IF(NX1.NE.NX2) GO TO 10                                           00006300
      DXQ= AX2-AX1                                                      00006310
      GO TO 13                                                          00006320
 10   IF(IX.NE.NX1) GO TO 11                                            00006330
      DXQ= GRID+X1-AX1                                                  00006340
      GO TO 13                                                          00006350
 11   IF(IX.NE.NX2) GO TO 12                                            00006360
      DXQ= GRID+AX2-X2                                                  00006370
      GO TO 13                                                          00006380
 12   DXQ=GRID                                                          00006390
C                                                                       00006400
C     START LOOP ON JY=NY1,NY2 ROWS OF THE RECEPTOR GRID.               00006410
 13   DO 2427 JY=NY1,NY2                                                00006420
      IF(NY1.NE.NY2) GO TO 20                                           00006430
      DY= AY2-AY1                                                       00006440
      GO TO 23                                                          00006450
 20   IF(JY.NE.NY1) GO TO 21                                            00006460
      DY= GRID+Y1-AY1                                                   00006470
      GO TO 23                                                          00006480
 21   IF(JY.NE.NY2) GO TO 22                                            00006490
      DY= GRID+AY2-Y2                                                   00006500
      GO TO 23                                                          00006510
 22   DY=GRID                                                           00006520
 23   SPLIT= DXQ*DY/(AREA*GRIDSQ)                                       00006530
C                                                                       00006540
C  LOOP FOR THE FIVE RECEPTORS AFFECTED BY EACH RECEPTOR GRID SQUARE    00006550
C    CONTAINING EMISSIONS.  THE RECEPTORS IN THE FOUR DOWNWIND SQUARES  00006560
C    AND IN THE SOURCE SQUARE ITSELF ARE AFFECTED.                      00006570
C                                                                       00006580
      DO 2426 L=1,5                                                     00006590
      NX= IX + ISIGNX*(ITABLE(L,IEPS)*ITABX + (L-1)*INCRX) - 4          00006600
      IF(NX.LT.1.OR.NX.GT.LX) GO TO 2426                                00006610
      NY= JY + ISIGNY*(ITABLE(L,IEPS)*ITABY + (L-1)*INCRY) - 4          00006620
      IF(NY.LT.1.OR.NY.GT.LY) GO TO 2426                                00006630
C                                                                       00006640
C     CALCULATE GROUND-LEVEL CONCENTRATIONS CONC (MICROGRAMS PER CUBIC  00006650
C     METER) AND SURFACE DEPOSITION FLUXES (MICROGRAMS PER SQUARE       00006660
C     METER PER HOUR) OF POLLUTANTS AT RECEPTOR IN COLUMN NX, ROW NY    00006670
C     OF THE RECEPTOR GRID DUE TO AREA SOURCE K.                        00006680
C                                                                       00006690
C     ISPEC = 1 OR 2 OR 3                                               00006700
      CINC1=RCA1(L)*EA(K,1)*SPLIT*STCONV                                00006710
      CONC(NX,NY,1)=CONC(NX,NY,1)+CINC1                                 00006720
      SDF(NX,NY,1)=SDF(NX,NY,1)+VD136*CINC1                             00006730
      IF(ISPEC.EQ.1) GO TO 2426                                         00006740
      IF(ISPEC.EQ.3) GO TO 2425                                         00006750
C                                                                       00006760
C     ISPEC = 2                                                         00006770
      CINC2=RCA2(L)*EA(K,2)*SPLIT*STCONV                                00006780
      CONC(NX,NY,2)=CONC(NX,NY,2)+CINC2                                 00006790
      SDF(NX,NY,2)=SDF(NX,NY,2)+VD236*CINC2                             00006800
      GO TO 2426                                                        00006810
C                                                                       00006820
C     ISPEC = 3                                                         00006830
 2425 CINC2=RCA2CT(L,K)*EA(K,1)*SPLIT*STCONV                            00006840
      CONC(NX,NY,2)=CONC(NX,NY,2)+CINC2                                 00006850
      SDF(NX,NY,2)=SDF(NX,NY,2)+VD236*CINC2                             00006860
C                                                                       00006870
2426  CONTINUE                                                          00006880
C     END LOOP ON L=1,5 CALCULATION GRID SQUARES WITH RECEPTORS.        00006890
C                                                                       00006900
2427  CONTINUE                                                          00006910
```

```
C     END LOOP ON JY=NY1,NY2 ROWS OF THE RECEPTOR GRID.
C
2428  CONTINUE
C     END LOOP ON IX=NX1,NX2 COLUMNS OF THE RECEPTOR GRID.
C
2429  CONTINUE
C     END LOOP ON K=1,NAS AREA SOURCES.
C
C
C
C *** POINT SOURCES.
C
C  HPEN= MINIMUM EFFECTIVE SOURCE HEIGHT NECESSARY FOR PLUME TO
C    PENETRATE INVERSION.
245   HPEN= PEN(ISCEN)*HMIX(ISCEN)
C
C
C  IF NO POINT SOURCES, SKIP POINT SOURCE CALCULATIONS.
      IF(NPS.LT.1) GO TO 603
C
C
C
C***  P O I N T   S O U R C E   C A L C U L A T I O N S  ***
C
C  LOOP THROUGH ALL POINT SOURCES.
      DO 600 I=1,NPS
      IF((NWDOPT.GT.1.AND.IWDOPT.GT.1).OR.NTOPT.EQ.2) GO TO 246
      IF(NPRINT.EQ.0) GO TO 246
      IF((I-1)/50*50.NE.I-1) GO TO 246
      WRITE(IWR,1005) TT,ISCEN,HMIX(ISCEN),HPEN
      WRITE(IWR,1007)
246   IPS=I
      IF(HP(I).GE.HMIX(ISCEN)) GO TO 600
      IRISE=2
      IBUOY=1
      EFF= 2.45*VP(I)*DP(I)*DP(I)*(TP(I)-TA(ISCEN))/TP(I)
      IF(EFF.LT.0.) EFF=1.0E-7
C
C  CALCULATE INVERSE WIND SPEED (UINV) AT THE PHYSICAL HEIGHT (HP(I))
C    OF POINT SOURCE I.  DO NOT CHANGE IF STACK HEIGHT IS LESS
C    THAN 10 METERS.
C
      UINV = 1./WS(ISCEN)
      IF(HP(I).GT.10.) UINV = UINV*((10./HP(I))**P(ISC))
      UPL=1./UINV
      UINV1=UINV/100.
C     DEFINE EMISSION RATES (SOURCE STRENGTHS) OF POLLUTANT SPECIES,
C      AND NONDIMENSIONAL DEPOSITION AND SEDIMENTATION PARAMETERS.
C
C     ISPEC = 1 OR 2 OR 3
      Q1=EP(I,1)
      VDC1=VD1*UINV1
      WC1=W1*UINV1
      V11=VDC1-0.5*WC1
      V21=VDC1-WC1
      IF(V21.EQ.0.) GO TO 48
      R11=V11/V21
      R21=0.5*WC1/V21
   48 IF(ISPEC.EQ.1) GO TO 50
C
C
C     ISPEC = 2 OR 3
      Q2=EP(I,2)
      VDC2=VD2*UINV1
      WC2=W2*UINV1
      V12=VDC2-0.5*WC2
      V22=VDC2-WC2
      IF(V22.EQ.0.) GO TO 49
      R12=V12/V22
      R22=0.5*WC2/V22
   49 IF(ISPEC.EQ.2) GO TO 51
C
C     ISPEC = 3
      IF(Q1.EQ.0.) Q1=1.E-6
      Q2Q1=Q2/Q1
      V13=V11-0.5*(WC1-WC2)
      IF(V21.EQ.0.) GO TO 50
      R13=V13/V21
      R23=0.5*WC2/V21
C
C     ISPEC = 1 OR 3
   50 UTAUC=TAUC*UPL
C
   51 KLID=0
C
C
C *** PEAK EFFECTIVE SOURCE HEIGHT CALCULATIONS.
C
      IF(ISC.LT.6) GO TO 247
C
C  DETERMINE WHETHER PLUME IS MOMENTUM-DOMINATED (IBUOY=0),
C                             OR BUOYANCY-DOMINATED (IBUOY=1).
C
C
C
C
      IF(ISC.EQ.6) BRIGC=115.28
      IF(ISC.EQ.7) BRIGC=87.14
      IF(VP(I).GT.BRIGC*(TP(I)-TA(ISCEN))*SQRT(TA(ISCEN))/TP(I)) IBUOY=0
      GO TO 249
247   AF= 21.425
      BF= 0.75
      IF(EFF.LT.55.) GO TO 248
      AF= 38.710
      BF= 0.6
248   IF(3.*VP(I)*DP(I).GT.AF*EFF**BF) IBUOY=0
249   CONTINUE
C
C  CALL SUBROUTINE RISE WITH IRISE=2 TO GET PEAK EFFECTIVE SOURCE
C    HEIGHT, ESH(2).
C
C     ************
      CALL RISE
C     ************
      IRISE=1
      IF(NPRINT.EQ.0) GO TO 1250
      IF(NWDOPT.LE.1.OR.IWDOPT.LE.1) WRITE(IWR,1010)
     1 I,XP(I),YP(I),EP(I,1),EP(I,2),HP(I),DP(I),VP(I),TP(I),
     2 PRL(1,IBUOY+1),PRL(2,IBUOY+1),DWL(IDWN),DWL(IDWN+1),UPL,ESH(2)
C
C  CALCULATE DISTANCE AT WHICH PLUME REACHES MAXIMUM HEIGHT (PEAK).
C
 1250 IF(IBUOY.EQ.0) GO TO 252
      IF(ISC.LT.6) GO TO 250
      PEAK=0.00207148/(UINV*SQRT(DTDZ(ISC-5)*9.8/TA(ISCEN)))
      GO TO 253
250   PEAK=0.001*XS
      GO TO 253
252   PEAK= 0.
      IF(ISC.GE.6) GO TO 253
      IF(ABS(VP(I)).LT..000001) GO TO 253
      PEAK=(0.004*UINV*(DP(I)*(VP(I) + 3./UINV))**2)/VP(I)
C
C  IF MAXIMUM EFFECTIVE SOURCE HEIGHT EXCEEDS HPEN, PLUME ESCAPES
C    THE MIXING LAYER, AND SOURCE IS IGNORED.
C
253   IF(ESH(2).GT.HPEN) GO TO 600
C
C  IF MAXIMUM EFFECTIVE SOURCE HEIGHT EXCEEDS MIXING HEIGHT BUT
C    NOT HPEN, PLUME DOES NOT ESCAPE THE MIXING LAYER, AND MAXIMUM
C    EFFECTIVE SOURCE HEIGHT IS SET EQUAL TO THE MIXING HEIGHT.
C
      IF(ESH(2).GT.HMIX(ISCEN)) ESH(2)=HMIX(ISCEN)
C
C
C  SET LIMITS (XMIN,XMAX,YMIN,YMAX) ON PORTION OF RECEPTOR GRID
C    EXAMINED FOR EACH SOURCE. THE EXTENT OF THIS PORTION DEPENDS
C    ON SOURCE LOCATION, GRID DIMENSIONS, AND WIND DIRECTION.
C
275   XMAX= XB2
      XMIN= XB1
      YMAX= YB2
      YMIN= YB1
      IF(XP(I)+60.0.LT.XB2) XMAX= XP(I) + 60.
      IF(XP(I)-60.0.GT.XB1) XMIN= XP(I) - 60.
      IF(YP(I)+60.0.LT.YB2) YMAX= YP(I) + 60.
      IF(YP(I)-60.0.GT.YB1) YMIN= YP(I) - 60.
      GO TO (280,285,290,295,300,305,310,315),IFLAG
  280 IF(WDPANG.GT.3.14)GOTO282
      IF(WDMANG.LT.0)GOTO284
      YMIN=YP(I)
      XL1=XP(I)+(YB2-YP(I))/TAN(WDPANG)
      IF(XL1.GT.XMIN)XMIN=XL1
      IF(XL1.GT.XP(I))XMIN=XP(I)
      XL2=XP(I)+(YB2-YP(I))/TAN(WDMANG)
      IF(XL2.LT.XMAX)XMAX=XL2
      IF(XL2.LT.XP(I))XMAX=XP(I)
      GOTO320
  282 YMIN=YP(I)+(XB1-XP(I))*TAN(WDPANG)
      XMAX=XP(I)+(YB2-YP(I))/TAN(WDMANG)
      GOTO320
  284 YMIN=YP(I)+(XB2-XP(I))*TAN(WDMANG)
      XMIN=XP(I)+(YB2-YP(I))/TAN(WDPANG)
      GOTO320
  285 XL1=XP(I)+(YB2-YP(I))/TAN(WDPANG)
      IF(XL1.GT.XMIN)XMIN=XL1
      IF(XL1.GT.XP(I))XMIN=XP(I)
      YL1=YP(I)+(XB2-XP(I))*TAN(WDMANG)
      IF(YL1.GT.YMIN)YMIN=YL1
      IF(YL1.GT.YP(I))YMIN=YP(I)
      GOTO320
  290 IF(WDPANG.GT.1.57.AND.WDMANG.LT.0.)GOTO292
      IF(WDPANG.GT.6.28.AND.WDMANG.LT.4.712)GOTO294
      XMIN=XP(I)
      YL1=YP(I)+(XB2-XP(I))*TAN(WDMANG)
      IF(YL1.GT.YMIN)YMIN=YL1
      IF(YL1.GT.YP(I))YMIN=YP(I)
      YL2=YP(I)+(XB2-XP(I))*TAN(WDPANG)
      IF(YL2.LT.YMAX)YMAX=YL2
      IF(YL2.LT.YP(I))YMAX=YP(I)
      GOTO320
  292 YMIN=YP(I)+(XB2-XP(I))*TAN(WDMANG)
      XMIN=XP(I)+(YB2-YP(I))/TAN(WDPANG)
      GOTO320
  294 XMIN=XP(I)+(YB1-YP(I))/TAN(WDMANG)
      YMAX=YP(I)+(XB2-XP(I))*TAN(WDPANG)
      GOTO320
  295 XL1=XP(I)+(YB1-YP(I))/TAN(WDMANG)
      IF(XL1.GT.XMIN)XMIN=XL1
      IF(XL1.GT.XP(I))XMIN=XP(I)
      YL2=YP(I)+(XB2-XP(I))*TAN(WDPANG)
      IF(YL2.LT.YMAX)YMAX=YL2
      IF(YL2.LT.YP(I))YMAX=YP(I)
      GOTO320
  300 IF(WDPANG.GT.6.28)GOTO302
      IF(WDMANG.LT.3.14)GOTO304
      YMAX=YP(I)
      XL1=XP(I)+(YB1-YP(I))/TAN(WDMANG)
      IF(XL1.GT.XMIN)XMIN=XL1
      IF(XL1.GT.XP(I))XMIN=XP(I)
      XL2=XP(I)+(YB1-YP(I))/TAN(WDPANG)
      IF(XL2.LT.XMAX)XMAX=XL2
      IF(XL2.LT.XP(I))XMAX=XP(I)
      GOTO320
  302 YMAX=YP(I)+(XB2-XP(I))*TAN(WDPANG)
      XMIN=XP(I)+(YB1-YP(I))/TAN(WDMANG)
      GOTO320
  304 YMAX=YP(I)+(XB1-XP(I))*TAN(WDMANG)
      XMAN=XP(I)+(YB1-YP(I))/TAN(WDPANG)
      GOTO320
  305 YL2=YP(I)+(XB1-XP(I))*TAN(WDMANG)
      IF(YL2.LT.YMAX)YMAX=YL2
      IF(YL2.LT.YP(I))YMAX=YP(I)
      XL2=XP(I)+(YB1-YP(I))/TAN(WDPANG)
      IF(XL2.LT.XMAX)XMAX=XL2
      IF(XL2.LT.XP(I))XMAX=XP(I)
      GOTO320
  310 IF(WDMANG.LT.1.57)GOTO312
      IF(WDPANG.GT.4.712)GOTO314
      XMAX=XP(I)
      YL1=YP(I)+(XB1-XP(I))*TAN(WDPANG)
      IF(YL1.GT.YMIN)YMIN=YL1
      IF(YL1.GT.YP(I))YMIN=YP(I)
      YL2=YP(I)+(XB1-XP(I))*TAN(WDMANG)
      IF(YL2.LT.YMAX)YMAX=YL2
      IF(YL2.LT.YP(I))YMAX=YP(I)
      GOTO320
  312 XL2=XP(I)+(YB2-YP(I))/TAN(WDMANG)
      IF(XL2.LT.XMAX)XMAX=XL2
      IF(XL2.LT.XP(I))XMAX=XP(I)
      YL1=YP(I)+(XB1-XP(I))*TAN(WDPANG)
      IF(YL1.GT.YMIN)YMIN=YL1
      IF(YL1.GT.YP(I))YMIN=YP(I)
      GOTO320
  314 XL2=XP(I)+(YB1-YP(I))/TAN(WDPANG)
      IF(XL2.LT.XMAX)XMAX=XL2
      IF(XL2.LT.XP(I))XMAX=XP(I)
      YL2=YP(I)+(XB1-XP(I))*TAN(WDMANG)
      IF(YL2.LT.YMAX)YMAX=YL2
      IF(YL2.LT.YP(I))YMAX=YP(I)
      GOTO320
  315 XL2=XP(I)+(YB2-YP(I))/TAN(WDMANG)
      IF(XL2.LT.XMAX)XMAX=XL2
      IF(XL2.LT.XP(I))XMAX=XP(I)
      YL1=YP(I)+(XB1-XP(I))*TAN(WDPANG)
      IF(YL1.GT.YMIN)YMIN=YL1
      IF(YL1.GT.YP(I))YMIN=YP(I)
      GOTO320
  320 IF(XMIN.GT.XB2.OR.XMAX.LT.XB1.OR.YMIN.GT.YB2.OR.YMAX.LT.YB1)
     1 GO TO 600
      IF(XMIN.LT.XB1) XMIN=XB1
      IF(XMAX.GT.XB2) XMAX=XB2
      IF(YMIN.LT.YB1) YMIN=YB1
      IF(YMAX.GT.YB2) YMAX=YB2
C
C  DETERMINE THE RANGE OF RECEPTOR GRID ROW AND COLUMN NUMBERS (LXMAX,
C     LXMIN,LYMAX,LYMIN) CORRESPONDING TO XMAX, ETC. ABOVE -
C
      LXMAX=(XMAX-XSWC)/GRID + 1.
      LXMIN= (XMIN-XSWC)/GRID + 1.
      LYMAX= (YMAX-YSWC)/GRID + 1.
      LYMIN= (YMIN-YSWC)/GRID + 1.
C
C     START LOOP ON ALL AFFECTED RECEPTORS.
      DO 500 IX=LXMIN,LXMAX
      XI=IX
      XG= XSWC + (XI-0.5)*GRID
      XD= XG - XP(I) + 0.00001
      XDSQ=XD*XD
      DO 500 JY=LYMIN,LYMAX
      YJ=JY
      YG= YSWC + (YJ-0.5)*GRID
      YD= YG - YP(I) + 0.00001
C  DSQ= SQUARE OF SOURCE-RECEPTOR DISTANCE. IF SOURCE-RECEPTOR DISTANCE
C     IS GREATER THAN 60 KM., RECEPTOR IS SKIPPED.
      DSQ= XDSQ + YD*YD
      IF(DSQ.GT.3600.) GO TO 500
      DELTA= ATAN(XD/YD)
      IF(DELTA.LT.0.) DELTA = DELTA + 3.1415927
      IF(XD.LT.0.) DELTA = DELTA + 3.1415927
      DELTA= ABS(DELTA - WVEC)
      IF(DELTA.GT.3.1415927) DELTA= ABS(6.2831853 - DELTA)
C  IF THE CROSSWIND ANGLE (DELTA) EXCEEDS A LIMITING VALUE WHICH
C     DEPENDS ON STABILITY CLASS (ANGLIM), THE RECEPTOR IS SKIPPED.
C       ANGLIM = 35,28,21,14,14,10.5,AND 7.0 DEGREES FOR 1-HOUR
C       FOR STABILITY CLASSES A, B, C, DD, DN, E, AND F RESPECTIVELY.
C
      IF(DELTA.GT.ANGLIM(ISC)) GO TO 500
C  DELTA IS THE ANGLE BETWEEN THE WIND VECTOR AND THE SOURCE-RECEPTOR
C     DIRECTION.  THE DOWNWIND DISTANCE USED IN THE GAUSSIAN PLUME
C     EQUATION IS=    DIST= SQRT(DSQ)*COS(DELTA).
      DIST=SQRT(DSQ)*COS(DELTA)
      IF(DIST.LT.0.002) GO TO 500
C
C
C *** DETERMINE PROBABILITY DENSITY OF CROSSWIND DISTRIBUTION
C      OF CONCENTRATIONS.
C
```

```
      XM=DIST*1000.
      IF(XM.GE.10000.) GO TO 323
      SIGY=CX1(ISC)*(XM**DX1(ISC))
      GO TO 324
  323 SIGY=CX2(ISC)*(XM**DX2(ISC))
  324 YM=XM*TAN(DELTA)
      DUMY=YM/SIGY
      ARG=0.5*DUMY*DUMY
      IF(ARG.GE.EXPMIN) GO TO 325
      EXPA=EXP(-ARG)
      GO TO 326
  325 EXPA=1.
  326 PYC=(A1B/SIGY)*EXPA
C
C
C *** DETERMINE PROBABILITY DENSITIES OF VERTICAL DISTRIBUTIONS
C     OF  SPECIES-1 AND SPECIES-2 POLLUTANT CONCENTRATIONS.
C
      IF(DIST.GT.D47) GO TO 330
C **** NEAR-SOURCE REGION (DIST .LE. D47).
C     CALCULATE QZC1 AND QZC2 FROM QZCAL (MODULE M=1).
C     ************
      CALL QZCAL
C     ************
      GO TO 350
C
  330 IF(DIST.LT.D80) GO TO 331
C **** WELL-MIXED REGION (DIST .GE. D80).
C     CALCULATE QZC1 AND QZC2 FROM QZCAL (MODULE M=2).
C     ************
      CALL QZCAL
C     ************
      GO TO 350
C
  331 IF(KLID.EQ.1) GO TO 337
C     CALCULATE QZC1 AND QZC2 FOR POLLUTANT SPECIES
C     AT DIST=D47 AND DIST=D80 FOR USE IN INTERPOLATION
C     IN PLUME-TRAPPING REGION.
      DUMX=DIST
      DIST=D47
C     ************
      CALL QZCAL
C     ************
      QZC11=QZC1
      IF(ISPEC.EQ.1) GO TO 332
      QZC21=QZC2
C
  332 DIST=D80
C     ************
      CALL QZCAL
C     ************
      QZC12=QZC1
      IRC1=1
      IF(QZC11.EQ.0.OR.QZC12.EQ.0.) IRC1=0
      IF(ISPEC.EQ.1) GO TO 333
      QZC22=QZC2
      IRC2=1
      IF(QZC21.EQ.0.OR.QZC22.EQ.0.) IRC2=0
C
  333 KLID=1
      DIST=DUMX
      IF(IRC1.EQ.0) GO TO 334
      DIFX1=ALOG(D80/D47)
      DIFC1=ALOG(QZC12/QZC11)
      GO TO 335
  334 DIFC1=QZC12-QZC11
  335 IF(ISPEC.EQ.1) GO TO 337
      IF(IRC2.EQ.0) GO TO 336
      DIFX2=ALOG(D80/D47)
      DIFC2=ALOG(QZC22/QZC21)
      GO TO 337
  336 DIFC2=QZC22-QZC21
C
C **** PLUME-TRAPPING REGION (D47 < DIST < D80).
C     CALCULATE QZC1 AND QZC2 BY LINEAR INTERPOLATION
C     (BETWEEN VALUES AT DIST=D47 AND DIST=D80) ON
C     A LOG-LOG PLOT OF QZC VERSUS DOWNWIND DISTANCE.
```

```
C     IF EITHER OF THE QZC VALUES AT D47 AND D80 ARE
C     ZERO, USE A LINEAR PLOT FOR INTERPOLATION.
  337 IF(IRC1.EQ.0) GO TO 338
      RATX1=ALOG(DIST/D47)/DIFX1
      QZC1L=ALOG(QZC11)+RATX1*DIFC1
      QZC1=EXP(QZC1L)
      GO TO 339
  338 RATX1=(DIST-D47)/D8047
      QZC1=QZC11+RATX1*DIFC1
  339 IF(ISPEC.EQ.1) GO TO 350
C
      IF(IRC2.EQ.0) GO TO 340
      RATX2=ALOG(DIST/D47)/DIFX2
      QZC2L=ALOG(QZC21)+RATX2*DIFC2
      QZC2=EXP(QZC2L)
      GO TO 350
  340 RATX2=(DIST-D47)/D8047
      QZC2=QZC21+RATX2*DIFC2
C
C
C
C     CALCULATE GROUND-LEVEL CONCENTRATIONS CONC (MICROGRAMS PER CUBIC
C     METER) AND SURFACE DEPOSITION FLUX SDF (MICROGRAMS PER SQUARE
C     METER PER HOUR) OF POLLUTANTS AT RECEPTOR IN COLUMN IX, ROW JY
C     OF THE RECEPTOR GRID DUE TO POINT SOURCE I.
C
C     ISPEC = 1 OR 2 OR 3
  350 C1=Q1*UINV*PYC*QZC1
      IF(NCSOPT.EQ.0) GO TO 355
      CALL WORST(IX,JY,C1)
      IF(NTOPT.GT.1) CONC(IX,JY,2)=CONC(IX,JY,2) + C1
  355 CINC1=C1*STCONV
      CONC(IX,JY,1)=CONC(IX,JY,1)+CINC1
      SDF(IX,JY,1)=SDF(IX,JY,1)+VD136*CINC1
      IF(ISPEC.EQ.1) GO TO 370
      IF(ISPEC.EQ.3) GO TO 360
C
C     ISPEC = 2
      C2=Q2*UINV*PYC*QZC2
      GO TO 365
C
C     ISPEC = 3
  360 C2=Q1*UINV*PYC*QZC2
C
  365 CINC2=C2*STCONV
      CONC(IX,JY,2)=CONC(IX,JY,2)+CINC2
      SDF(IX,JY,2)=SDF(IX,JY,2)+VD236*CINC2
  370 CONTINUE
C
500   CONTINUE
C     END LOOP ON ALL AFFECTED RECEPTORS.
C
600   CONTINUE
C     END LOOP ON ALL POINT SOURCES.
C
C
C
C *** PRINT OUTPUT.
C
C     OUTPUT AT END OF EACH SCENARIO OR SUB-SCENARIO
C
C     TIME AVERAGING:  NTOPT=2 OR 3
C       AT END OF EACH SCENARIO, CALL WOROUT TO PRINT OUTPUT FOR
C         NCSOPT OPTION.
C       IF LAST SCENARIO, CALL OUTMOD TO PRINT OUTPUT FOR NLIST, NTAPE,
C         AND NARRAY OPTIONS.  CALL MAXOUT TO PRINT OUTPUT FOR NMAX.
C         OTHERWISE, GO TO 100 FOR THE NEXT SCENARIO.
C
C     NO TIME AVERAGING: NTOPT=1
C       AT END OF EACH SCENARIO (OR SUB-SCENARIO WHEN NWDOPT.GT.1),
C         CALL OUTMOD TO PRINT OUTPUT FOR NCSOPT, NLIST, NTAPE,
C         AND NARRAY OPTIONS.
C       IF LAST SCENARIO (AND LAST SUB-SCENARIO WHEN NWDOPT.GT.1),
C         CALL MAXOUT TO PRINT OUTPUT FOR NMAX OPTION.
C         OTHERWISE, GO TO 100 FOR THE THE NEXT SCENARIO OR SUB-SCENARIO
C
  603 IF(NTOPT.EQ.1) GO TO 620
```

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C                                                                       00011540
C     TIME AVERAGING: NTOPT=2 OR 3                                      00011550
C                                                                       00011560
      IF(NCSOPT.GT.0) CALL WOROUT                                       00011570
      IF(ISCEN.NE.NSCEN) GO TO 100                                      00011580
      CALL OUTMOD                                                       00011590
      GO TO 999                                                         00011600
C                                                                       00011610
C     NO TIME AVERAGING: NTOPT=1                                        00011620
C                                                                       00011630
  620 CALL OUTMOD                                                       00011640
      IF(ISCEN.NE.NSCEN) GO TO 100                                      00011650
      IF(NWDOPT.LE.1) GO TO 999                                         00011660
      IF(IWDOPT.LT.4) GO TO 100                                         00011670
C                                                                       00011680
  999 IF(NMAX.GT.0) CALL MAXOUT                                         00011690
C                                                                       00011700
      STOP                                                              00011710
C                                                                       00011720
C                                                                       00011730
 1005 FORMAT(1H1,45X,'POLLUTION EPISODIC MODEL'///4X,'OUTPUT:  ',20A4// 00011740
     14X,'SCENARIO',I2,4X,'POINT SOURCE PLUME RISE CALCULATIONS'/       00011750
     221X,'MIXING HEIGHT: HMIX=',F7.2,' M'/                             00011760
     321X,'IF MAXIMUM EFFECTIVE SOURCE HEIGHT IS GREATER THAN ',F7.1,   00011770
     4' M, THE SOURCE IS IGNORED'/)                                     00011780
 1007 FORMAT(14X,'SOURCE',8X,'EMISSION RATES',61X,'WIND SPEED AT',4X,   00011790
     1 'MAXIMUM'/' POINT',6X,'COORDINATES',4X,'POL-1',6X,'POL-2',4X,    00011800
     2 'HEIGHT  DIAMETER  EXIT VEL  EXIT TEMP',6X,'DOMINANT',5X,        00011810
     3 'STACK HEIGHT',4X,'EFFECTIVE'/' SOURCE',3X,'X(KM)',4X,'Y(KM)',3X,00011820
     4 '(G/S)',6X,'(G/S)',5X,'(M)',6X,'(M)',7X,'(M/S)',4X,'(DEG K)',6X, 00011830
     5 'INFLUENCE',8X,'(M/S)',6X,'SOURCE HEIGHT(M)'/)                   00011840
 1010 FORMAT(1X,I4,2X,F8.2,1X,F8.2,2X,F8.2,2X,F8.2,2X,F7.2,3X,F6.3,3X,  00011850
     1 F8.3,3X,F7.2,2X,2A4,1X,2A4,3X,F7.3,8X,F8.2)                      00011860
      END                                                               00011870
C                                                                       00011880
C                                                                       00011890
      SUBROUTINE QZCAL                                                  00011900
C                    SUBROUTINE QZCAL  (VERSION 82360), PART OF PEM.    00011910
C                                                                       00011920
C                                                                       00011930
C  SUBROUTINE QZCAL CALCULATES QZC1 AND QZC2,  REPRESENTING THE         00011940
C     PROBABLITY DENSITIES OF VERTICAL DISTRIBUTIONS OF CONCENTRATIONS  00011950
C     OF POLLUTANT SPECIES 1 AND 2, RESPECTIVELY, AT A GIVEN            00011960
C     DISTANCE DOWNWIND OF A POINT SOURCE.                              00011970
C                                                                       00011980
C                                                                       00011990
C *** PEM  ALGORITHMS AND PROGRAM DEVELOPMENT    ---DECEMBER 1982       00012000
C                                                                       00012010
C     K. SHANKAR RAO, PHYSICAL RESEARCH SCIENTIST                       00012020
C     ATMOSPHERIC TURBULENCE AND DIFFUSION LABORATORY (ATDL)            00012030
C     NATIONAL OCEANIC AND ATMOSPHERIC ADMINISTRATION (NOAA)            00012040
C     U.S. DEPARTMENT OF COMMERCE, P.O. BOX - E                         00012050
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C             FTS: 626-1238                                             00012080
C                                                                       00012090
C     ( THIS WORK WAS DONE UNDER AN INTERAGENCY AGREEMENT               00012100
C     BETWEEN THE ENVIRONMENTAL PROTECTION AGENCY AND THE               00012110
C     NATIONAL OCEANIC AND ATMOSPHERIC ADMINISTRATION )                 00012120
C                                                                       00012130
C                                                                       00012140
C                                                                       00012150
      COMMON/PEMCOM/CONC(50,50,2),SDF(50,50,2),  TT(20),                00012160
     1 XP(300),YP(300),EP(300,2),HP(300),DP(300),VP(300),TP(300),       00012170
     2 XA(50),YA(50),EA(50,2),SIZE(50),                                 00012180
     3 WD(24),WS(24),TA(24),HMIX(24),PEN(24),                           00012190
     4 AX(7,3),BX(7,3),P(7),SCLAB(7),DTDZ(2),  SECTAN(16),              00012200
     5 XSWC,YSWC,GRID,LX,LY,    A(2),B(2),POLNAM(3,2),CALNAM(7,2),      00012210
     6 ITA,IRD,IWR,IDSK,          D80,D47,D8047,DIST,DELTA,             00012220
     7 ESH(2),PEAK,IBUOY,IRISE,IDWN,EFF,XS,    UINV,WVEC,               00012230
     8 NAS,NPS,INDEX,IGRID,IAV,ISCEN,IWDOPT,IWD,ISC,IPS,                00012240
     9 NTOPT,NWDOPT,NWSOPT,NSCEN,NLIST,NARRAY,NTAPE,NCSOPT,NMAX,        00012250
     * NSTDWN,INTER,NPRINT                                              00012260
C                                                                       00012270
      COMMON/PARM1/NPOL,ICT,VD1,W1,VD2,W2,TAUC                          00012280
      COMMON/PARM1A/GAMMA                                               00012290
      COMMON/PARM2/ISPEC,UTAUC,Q2Q1,XCT,EXCT                            00012300
      COMMON/PARM3/HC,VDC1,WC1,VDC2,WC2                                 00012310
      COMMON/PARM4/V11,V21,V12,V22,V13                                  00012320
      COMMON/PARM5/D11,D21,D12,D22,D31,D32,D33,D6                       00012330
      COMMON/PARM6/R11,R21,R12,R22,R13,R23,R31,R41,R32,R42              00012340
      COMMON/PARM7/QZC1,QZC2                                            00012350
      COMMON/BLOCK1/PI,SQPI,SQRT2,A1B,A1C                               00012360
      COMMON/BLOCK2/AI,BI,EPSABS,EPSREL,LW,NIW                          00012370
      COMMON/EXPCHK/EXPMAX,EXPMIN,ETAMAX                                00012380
      EXTERNAL FUN1                                                     00012390
      REAL*8 FUN1                                                       00012400
      REAL*8 WORK(800),AI,BI,EPSABS,EPSREL,RESULT,ABSERR                00012410
      DIMENSION IW(102)                                                 00012420
C                                                                       00012430
C                                                                       00012440
C                                                                       00012450
      IF(DIST.GE.PEAK) GO TO 5                                          00012460
C                                                                       00012470
C  CALL SUBROUTINE RISE FOR EFFECTIVE SOURCE HEIGHT AT DOWNWIND         00012480
C    DISTANCE = DIST, LESS THAN DISTANCE TO MAXIMUM HEIGHT (PEAK).      00012490
C     ************                                                      00012500
      CALL RISE                                                         00012510
C     ************                                                      00012520
      HGT= ESH(1)                                                       00012530
      GO TO 6                                                           00012540
C                                                                       00012550
C  USE MAXIMUM EFFECTIVE SOURCE HEIGHT, SINCE DOWNWIND DISTANCE         00012560
C    EXCEEDS THE DISTANCE TO MAXIMUM HEIGHT.                            00012570
    5 HGT= ESH(2)                                                       00012580
    6 JD=2                                                              00012590
      IF(DIST.LT.0.5) JD=1                                              00012600
      IF(DIST.GT.5.0) JD=3                                              00012610
C                                                                       00012620
C                                                                       00012630
      HL=HMIX(ISCEN)                                                    00012640
      X=DIST                                                            00012650
      XM=X*1000.                                                        00012660
      SIGZ= AX(ISC,JD)*(XM**BX(ISC,JD))                                 00012670
      IF(SIGZ.GT.5000.) SIGZ=5000.                                      00012680
      SZ=SIGZ                                                           00012690
      C2=SQRT2*SZ                                                       00012700
      HC=HGT/C2                                                         00012710
      XC=XM/C2                                                          00012720
C                                                                       00012730
C     ISPEC = 1 OR 2 OR 3                                               00012740
      D31=2.*V11*XC                                                     00012750
      D11=WC1*XC                                                        00012760
      D21=D11*D11                                                       00012770
      R31=1.+2.*D21                                                     00012780
      R41=2.*D11/SQPI                                                   00012790
      IF(ISPEC.EQ.1) GO TO 9                                            00012800
C                                                                       00012810
C     ISPEC = 2 OR 3                                                    00012820
      D32=2.*V12*XC                                                     00012830
      D12=WC2*XC                                                        00012840
      D22=D12*D12                                                       00012850
      R32=1.+2.*D22                                                     00012860
      R42=2.*D12/SQPI                                                   00012870
      IF(ISPEC.EQ.2) GO TO 10                                           00012880
C                                                                       00012890
C     ISPEC = 3                                                         00012900
      D33=2.*V13*XC                                                     00012910
      D6=4.*SQPI*(V21-V22)*XC                                           00012920
C                                                                       00012930
    9 TCC=UTAUC/C2                                                      00012940
   10 IF(ICT.EQ.0) XCT=0.                                               00012950
      IF(ICT.EQ.1) XCT=XC/TCC                                           00012960
      EXCT=EXP(-XCT)                                                    00012970
C                                                                       00012980
      TERM1=0.                                                          00012990
      TERM2=0.                                                          00013000
      TERM3=0.                                                          00013010
C                                                                       00013020
      DUM1=D47+0.001                                                    00013030
      DUM2=D80-0.001                                                    00013040
      IF(X.LT.DUM1) GO TO 100                                           00013050
      IF(X.GT.DUM2) GO TO 200                                           00013060
C                                                                       00013070
```

```
   11 QZC1=0.0
      QZC2=0.0
      RETURN
C
C
C **** NEAR-SOURCE REGION (X .LE. D47).
C
  100 M=1
      A1=A1B/SZ
      C3=HC*HC
      IF(C3.GE.EXPMIN) GO TO 11
      A2=1./EXP(C3)
C
C     ISPEC = 1 OR 2 OR 3
C     SPECIES-1 (PRIMARY) POLLUTANT: GAS OR PARTICLES.
      ETA1=HC+D31
      ETA1SQ=ETA1*ETA1
      IF(ETA1SQ.GT.EXPMAX) CALL ARGCHK(ETA1,ETA1SQ)
      B11=EXP(ETA1SQ)*ERFC(ETA1)
      ALPHA1=A1C*D31*B11
      SUM=2.-ALPHA1
      IF(SUM) 115,115,116
  115 G21P=0.0
      GO TO 120
  116 IF(WC1.EQ.0.) GO TO 117
      BETA1=-2.*D11*HC+D21
      CALL EXPO(-BETA1,EBT1)
      GO TO 118
  117 EBT1=1.0
  118 G21P=EXCT*EBT1*A2*SUM
  120 QZC1=A1*G21P
      IF(ISPEC.EQ.1) RETURN
C
C
C     ISPEC = 2 OR 3
C     SPECIES-2 (SECONDARY) POLLUTANT: GAS OR PARTICLES.
      ETA2=HC+D32
      ETA2SQ=ETA2*ETA2
      IF(ETA2SQ.GT.EXPMAX) CALL ARGCHK(ETA2,ETA2SQ)
      B12=EXP(ETA2SQ)*ERFC(ETA2)
      ALPHA2=A1C*D32*B12
      SUM1=2.-ALPHA2
      IF(ISPEC.EQ.3) GO TO 145
C
C     ISPEC = 2
      IF(SUM1) 135,135,140
  135 G22P=0.0
      QZC2=0.0
      RETURN
  140 IF(WC2.EQ.0.) GO TO 141
      BETA2=-2.*D12*HC+D22
      CALL EXPO(-BETA2,EBT2)
      GO TO 142
  141 EBT2=1.0
  142 G22P=EBT2*A2*SUM1
      QZC2=A1*G22P
      RETURN
C
C     ISPEC = 3
  145 TERM1=(Q2Q1+GAMMA)*A2*SUM1
C
      ETA3=HC+D33
      ETA3SQ=ETA3*ETA3
      IF(ETA3SQ.GT.EXPMAX) CALL ARGCHK(ETA3,ETA3SQ)
      B13=EXP(ETA3SQ)*ERFC(ETA3)
      ALPHA3=A1C*D33*B13
      TERM2=-GAMMA*EXCT*A2*(2.-ALPHA3)
C
      IF(V21.EQ.V22) GO TO 150
C     COMPUTE INTEGRAL FUNC=F1(XC,0.;HC); FUN1 IS THE INTEGRAND FUNCTION
      CALL D01AJF(FUN1,AI,BI,EPSABS,EPSREL,RESULT,
     1   ABSERR,WORK,LW,IW,NIW,IFAIL)
      RES=RESULT
      FUNC=RES/PI
      TERM3=-GAMMA*D6*FUNC
C
  150 SUMT=TERM1+TERM2+TERM3
```

```
      IF(SUMT) 155,155,160
  155 G22P=0.0
      QZC2=0.0
      RETURN
  160 IF(HC2.EQ.0.) GO TO 161
      BETA2=-2.*D12*HC+D22
      CALL EXPO(-BETA2,EBT2)
      GO TO 162
  161 EBT2=1.0
  162 G22P=EBT2*SUMT
      QZC2=A1*G22P
      RETURN
C
C
C **** WELL-MIXED REGION (X .GE. D80).
C
C     IN THIS REGION, THE CONCENTRATION BELOW THE MIXING HEIGHT IS
C     UNIFORM REGARDLESS OF THE SOURCE OR RECEPTOR HEIGHTS BECAUSE
C     OF THOROUGH MIXING OF POLLUTANT BETWEEN THE GROUND AND THE
C     MIXING HEIGHT.
C
  200 M=2
      A1A=1000./HL
      CALL PSG4P(G41P,G42P)
      QZC1=A1A*G41P
      IF(ISPEC.EQ.1) RETURN
      QZC2=A1A*G42P
      RETURN
      END
C
C
      SUBROUTINE PSG4P(G41P,G42P)
C                       SUBROUTINE PSG4P (VERSION 82360), PART OF PEM.
C
C
C     THIS SUBROUTINE CALCULATES AND RETURNS VALUES OF G41P AND G42P.
C     THESE ARE NONDIMENSIONAL VERTICALLY-INTEGRATED PROBABILITY
C     DENSITY FUNCTIONS USED IN THE WELL-MIXED REGION CONCENTRATION
C     ALGORITHMS FOR SPECIES-1 AND SPECIES-2, RESPECTIVELY, DOWNWIND
C     OF A POINT SOURCE.  THESE FUNCTIONS ARE INDEPENDENT OF BOTH
C     SOURCE HEIGHT AND RECEPTOR HEIGHT.  THIS SUBROUTINE IS
C     USED BY BOTH POINT AND AREA SOURCES.  FOR AREA SOURCES,
C     G41P AND G42P REPRESENT SUSPENSION RATIOS OF POLLUTANTS.
C
C
C
C *** PEM ALGORITHMS AND PROGRAM DEVELOPMENT: --- DECEMBER 1982
C
C     K. SHANKAR RAO, PHYSICAL RESEARCH SCIENTIST
C     ATMOSPHERIC TURBULENCE AND DIFFUSION LABORATORY (ATDL)
C     NATIONAL OCEANIC AND ATMOSPHERIC ADMINISTRATION (NOAA)
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C
C     ( THIS WORK WAS DONE UNDER AN INTERAGENCY AGREEMENT
C     BETWEEN THE ENVIRONMENTAL PROTECTION AGENCY AND THE
C     NATIONAL OCEANIC AND ATMOSPHERIC ADMINISTRATION )
C
C
C
      EXTERNAL FUN2
      REAL*8 FUN2
      REAL*8 WORK(800),AI,BI,EPSABS,EPSREL,RESULT,ABSERR
      DIMENSION IW(102)
      COMMON/PARM1A/GAMMA
      COMMON/PARM2/ISPEC,UTAUC,Q2Q1,XCT,EXCT
      COMMON/PARM4/V11,V21,V12,V22,V13
      COMMON/PARM5/D11,D21,D12,D22,D31,D32,D33,D6
      COMMON/PARM6/R11,R21,R12,R22,R13,R23,R31,R41,R32,R42
      COMMON/BLOCK1/PI,SQPI,SQRT2,A1B,A1C
      COMMON/BLOCK2/AI,BI,EPSABS,EPSREL,LW,NIW
      COMMON/EXPCHK/EXPMAX,EXPMIN,ETAMAX
C
C
C     ISPEC = 1 OR 2 OR 3
```

```
C***** SPECIES-1 (PRIMARY) POLLUTANT: GAS OR PARTICLES.                 00014620
C                                                                       00014630
      IF(D21.GT.EXPMAX) CALL ARGCHK(D11,D21)                            00014640
      B11=EXP(D21)*ERFC(D11)                                            00014650
      IF(V21.EQ.0.) GO TO 201                                           00014660
      D31SQ=D31*D31                                                     00014670
      IF(D31SQ.GT.EXPMAX) CALL ARGCHK(D31,D31SQ)                        00014680
      SUM=R11*(EXP(D31SQ)*ERFC(D31))-R21*B11                            00014690
      GO TO 202                                                         00014700
  201 SUM=R31*B11-R41                                                   00014710
  202 IF(SUM.LT.0.) SUM=0.0                                             00014720
      G41P=EXCT*EXP(-D21)*SUM                                           00014730
      IF(ISPEC.EQ.1) RETURN                                             00014740
C                                                                       00014750
C     ISPEC = 2 OR 3                                                    00014760
C***** SPECIES-2 (SECONDARY) POLLUTANT: GAS OR PARTICLES.               00014770
C                                                                       00014780
      IF(D22.GT.EXPMAX) CALL ARGCHK(D12,D22)                            00014790
      B12=EXP(D22)*ERFC(D12)                                            00014800
      IF(V22.EQ.0.) GO TO 203                                           00014810
      D32SQ=D32*D32                                                     00014820
      IF(D32SQ.GT.EXPMAX) CALL ARGCHK(D32,D32SQ)                        00014830
      SUM1=R12*(EXP(D32SQ)*ERFC(D32))-R22*B12                           00014840
      GO TO 204                                                         00014850
  203 SUM1=R32*B12-R42                                                  00014860
  204 IF(ISPEC.EQ.3) GO TO 205                                          00014870
C                                                                       00014880
C     ISPEC = 2                                                         00014890
      IF(SUM1.LT.0.) SUM1=0.0                                           00014900
      G42P=EXP(-D22)*SUM1                                               00014910
      RETURN                                                            00014920
C                                                                       00014930
C     ISPEC = 3                                                         00014940
  205 TERM1=(Q2Q1+GAMMA)*SUM1                                           00014950
C                                                                       00014960
      IF(V21.EQ.0.) GO TO 206                                           00014970
      D33SQ=D33*D33                                                     00014980
      IF(D33SQ.GT.EXPMAX) CALL ARGCHK(D33,D33SQ)                        00014990
      SUM2=R13*(EXP(D33SQ)*ERFC(D33))-R23*B12                           00015000
      GO TO 207                                                         00015010
  206 SUM2=R32*B12-R42                                                  00015020
  207 TERM2=-GAMMA*EXCT*SUM2                                            00015030
C                                                                       00015040
      IF(V21.EQ.V22) GO TO 208                                          00015050
C     COMPUTE INTEGRAL FUNC=F2(XC); FUN2 IS THE INTEGRAND FUNCTION.     00015060
      CALL D01AJF(FUN2,AI,BI,EPSABS,EPSREL,RESULT,                      00015070
     1  ABSERR,WORK,LW,IW,NIW,IFAIL)                                    00015080
      RES=RESULT                                                        00015090
      FUNC=RES/(2.*PI)                                                  00015100
      TERM3=-GAMMA*D6*FUNC                                              00015110
      GO TO 209                                                         00015120
  208 TERM3=0.0                                                         00015130
C                                                                       00015140
  209 SUMT=TERM1+TERM2+TERM3                                            00015150
      IF(SUMT.LT.0.) SUMT=0.0                                           00015160
      G42P=EXP(-D22)*SUMT                                               00015170
      RETURN                                                            00015180
      END                                                               00015190
C                                                                       00015200
C                                                                       00015210
      DOUBLE PRECISION FUNCTION FUN1(T)                                 00015220
      REAL*8 T,TERM1,TERM2,TERM3
C                         REAL*8 FUNCTION FUN1(VERSION 82360), PART OF PEM. 00015230
C                                                                       00015240
C                                                                       00015250
C     INTEGRAND FUNCTION USED IN THE NUMERICAL INTEGRATION IN SUBROUTINE00015260
C     QZCAL (FOR POINT SOURCES) IS DEFINED HERE.                        00015270
C                                                                       00015280
C                                                                       00015290
C     PEM ALGORITHMS AND PROGRAM DEVELOPMENT: DECEMBER 1982             00015300
C     K. SHANKAR RAO                                                    00015310
C     NOAA-ATDL, P.O. BOX-E                                             00015320
C     OAK RIDGE, TENN 37830                                             00015330
C                                                                       00015340
C                                                                       00015350
      COMMON/PARM2/ISPEC,UTAUC,Q2Q1,XCT,EXCT                            00015360
      COMMON/PARM3/HC,VDC1,WC1,VDC2,WC2                                 00015370
      COMMON/PARM5/D11,D21,D12,D22,D31,D32,D33,D6
      COMMON/BLOCK1/PI,SQPI,SQRT2,A1B,A1C
      COMMON/EXPCHK/EXPMAX,EXPMIN,ETAMAX
C
C
      SQT=SQRT(T)
      SQ1T=SQRT(1.-T)
      HC1=HC/SQT
C
      ARG1= -(HC1*HC1)-(T*XCT)
      CALL EXPO(ARG1,EXP1)
      IF(EXP1.EQ.0.) GO TO 10
      TERM1= EXP1/(SQT*SQ1T)
C
      ETA4=HC1+D33*SQT
      ETA4SQ=ETA4*ETA4
      IF(ETA4SQ.GT.EXPMAX) CALL ARGCHK(ETA4,ETA4SQ)
      TERM2A= EXP(ETA4SQ)*ERFC(ETA4)
      HC1SQ=HC1*HC1
      IF(HC1SQ.GT.EXPMAX) CALL ARGCHK(HC1,HC1SQ)
      TERM2= 1. -SQPI*(ETA4-HC1)*TERM2A
      IF(TERM2.LE.0.) GO TO 10
C
      ETA5=D32*SQ1T
      ETA5SQ=ETA5*ETA5
      IF(ETA5SQ.GT.EXPMAX) CALL ARGCHK(ETA5,ETA5SQ)
      TERM3=1.-SQPI*ETA5*(EXP(ETA5SQ)*ERFC(ETA5))
      IF(TERM3.LE.0.) GO TO 10
C
      FUN1=TERM1*TERM2*TERM3
      GO TO 11
   10 FUN1=0.0
   11 RETURN
      END
C
C
      DOUBLE PRECISION FUNCTION FUN2(T)
      REAL*8 T
C                        REAL*8 FUNCTION FUN2 (VERSION 82360), PART OF PEM.
C
C
C     INTEGRAND FUNCTION USED IN THE NUMERICAL INTEGRATION IN SUBROUTINE
C     PSG4P (FOR POINT AND AREA SOURCES) IS DEFINED HERE.
C
C
C     PEM ALGORITHMS AND PROGRAM DEVELOPMENT: DECEMBER 1982
C     K. SHANKAR RAO
C     NOAA-ATDL, P.O. BOX-E
C     OAK RIDGE, TENN 37830
C
C
      COMMON/PARM2/ISPEC,UTAUC,Q2Q1,XCT,EXCT
      COMMON/PARM4/V11,V21,V12,V22,V13
      COMMON/PARM5/D11,D21,D12,D22,D31,D32,D33,D6
      COMMON/PARM6/R11,R21,R12,R22,R13,R23,R31,R41,R32,R42
      COMMON/BLOCK1/PI,SQPI,SQRT2,A1B,A1C
      COMMON/EXPCHK/EXPMAX,EXPMIN,ETAMAX
C
C
      SQT=SQRT(T)
      SQ1T=SQRT(1.-T)
      ETA4=D33*SQT
      ETA5=D32*SQ1T
      ETA6=D12*SQ1T
      ETA6SQ=ETA6*ETA6
      IF(ETA6SQ.GT.EXPMAX) CALL ARGCHK(ETA6,ETA6SQ)
C
      ARG1=T*XCT
      EXP1=EXP(-ARG1)
      TERM1=EXP1/SQT
C
      IF(ETA4.EQ.0.) GO TO 10
      ETA4SQ=ETA4*ETA4
      IF(ETA4SQ.GT.EXPMAX) CALL ARGCHK(ETA4,ETA4SQ)
      TERM2=1.-SQPI*ETA4*(EXP(ETA4SQ)*ERFC(ETA4))
      IF(TERM2.LT.0.) TERM2=0.
      GO TO 11
   10 TERM2=1.
C                                                                       00016140
   11 IF(V22.EQ.0.) GO TO 12                                            00016150
      ETA5SQ=ETA5*ETA5                                                  00016160
      IF(ETA5SQ.GT.EXPMAX) CALL ARGCHK(ETA5,ETA5SQ)                     00016170
      T3A=EXP(ETA5SQ)*ERFC(ETA5)                                        00016180
      T3B=EXP(ETA6SQ)*ERFC(ETA6)                                        00016190
      TERM3=R12*T3A-R22*T3B                                             00016200
      IF(TERM3.LT.0.) TERM3=0.                                          00016210
      GO TO 13                                                          00016220
C                                                                       00016230
   12 T3A=(1.+2.*ETA6SQ)*(EXP(ETA6SQ)*ERFC(ETA6))                       00016240
      T3B=2.*ETA6/SQPI                                                  00016250
      TERM3=T3A-T3B                                                     00016260
      IF(TERM3.LT.0.) TERM3=0.                                          00016270
C                                                                       00016280
   13 FUN2=TERM1*TERM2*TERM3                                            00016290
      RETURN                                                            00016300
      END                                                               00016310
C                                                                       00016320
C                                                                       00016330
      DOUBLE PRECISION FUNCTION FUN3(T)                                 00016340
      REAL*8 T                                                          00016350
C                     REAL*8 FUNCTION FUN3 (VERSION 82360), PART OF PEM. 00016360
C                                                                       00016370
C                                                                       00016380
C     INTEGRAND FUNCTION USED IN THE NUMERICAL INTEGRATION FOR AREA     00016390
C     SOURCES IN MAIN PROGRAM IS DEFINED HERE.                          00016400
C                                                                       00016410
C                                                                       00016420
C     PEM ALGORITHMS AND PROGRAM DEVELOPMENT: DECEMBER 1982             00016430
C     K. SHANKAR RAO                                                    00016440
C     NOAA-ATDL, P.O. BOX - E                                           00016450
C     OAK RIDGE, TENN 37830                                             00016460
C                                                                       00016470
C                                                                       00016480
      COMMON/PARM2/ISPEC,UTAUC,Q2Q1,XCT,EXCT                            00016490
      COMMON/PARM2A/AA,BA                                               00016500
      COMMON/PARM3/HC,VDC1,WC1,VDC2,WC2                                 00016510
      COMMON/PARM4/V11,V21,V12,V22,V13                                  00016520
      COMMON/PARM6/R11,R21,R12,R22,R13,R23,R31,R41,R32,R42              00016530
      COMMON/BLOCK1/PI,SQPI,SQRT2,A1B,A1C                               00016540
      COMMON/EXPCHK/EXPMAX,EXPMIN,ETAMAX                                00016550
C                                                                       00016560
C                                                                       00016570
      DN=SQRT2*AA                                                       00016580
      BA1=1.-BA                                                         00016590
      UTBA1=(UTAUC)**BA1                                                00016600
      P1=2.*V11*UTBA1/DN                                                00016610
      TBA1=T**BA1                                                       00016620
      ETA1=P1*TBA1                                                      00016630
      ETA1SQ=ETA1*ETA1                                                  00016640
      IF(ETA1SQ.GT.EXPMAX) CALL ARGCHK(ETA1,ETA1SQ)                     00016650
      TERM=EXP(ETA1SQ)*ERFC(ETA1)                                       00016660
      EXP1=EXP(-T)                                                      00016670
C                                                                       00016680
      IF(WC1.NE.0.) GO TO 11                                            00016690
   10 SUM=TERM                                                          00016700
      GO TO 13                                                          00016710
C                                                                       00016720
   11 IF(V21.EQ.0.) GO TO 12                                            00016730
      P2=WC1*UTBA1/DN                                                   00016740
      B1=P2*TBA1                                                        00016750
      B1SQ=B1*B1                                                        00016760
      IF(B1SQ.GT.EXPMAX) CALL ARGCHK(B1,B1SQ)                           00016770
      SUM=EXP(-B1SQ)*(R11*TERM-R21*(EXP(B1SQ)*ERFC(B1)))               00016780
      GO TO 13                                                          00016790
C                                                                       00016800
   12 RF1=1.+2.*ETA1SQ                                                  00016810
      RS1=2.*ETA1/SQPI                                                  00016820
      SUM=EXP(-ETA1SQ)*(RF1*TERM-RS1)                                   00016830
C                                                                       00016840
   13 IF(SUM.LT.0.) SUM=0.0                                             00016850
      FUN3=EXP1*SUM/VDC1                                                00016860
      RETURN                                                            00016870
      END                                                               00016880
C                                                                       00016890
```

```
C                                                                       00016900
      SUBROUTINE EXPO(BX,EX)                                            00016910
C                       SUBROUTINE EXPO (VERSION 82360), PART OF PEM.   00016920
C                                                                       00016930
C                                                                       00016940
C     GIVEN THE ARGUMENT BX, SUBROUTINE EXPO CALCULATES AND             00016950
C     RETURNS EX=EXP(BX).  EXPO LIMITS THE ARGUMENT TO AVOID            00016960
C     OVERFLOW/UNDERFLOW ERRORS.                                        00016970
C                                                                       00016980
C                                                                       00016990
C     PEM ALGORITHMS AND PROGRAM DEVELOPMENT: DECEMBER 1982             00017000
C     K. SHANKAR RAO                                                    00017010
C     NOAA-ATDL, P.O. BOX-E                                             00017020
C     OAK RIDGE, TENN 37830                                             00017030
C                                                                       00017040
C                                                                       00017050
      COMMON/EXPCHK/EXPMAX,EXPMIN,ETAMAX                                00017060
C                                                                       00017070
C                                                                       00017080
      BXABS=ABS(BX)                                                     00017090
      IF(BX) 5,10,15                                                    00017100
    5 IF(BXABS-EXPMIN) 6,7,7                                            00017110
    6 EX=EXP(BX)                                                        00017120
      GO TO 20                                                          00017130
    7 EX=0.                                                             00017140
      GO TO 20                                                          00017150
   10 EX=1.                                                             00017160
      GO TO 20                                                          00017170
   15 IF(BXABS.GT.EXPMAX) BXABS=EXPMAX                                  00017180
      EX=EXP(BXABS)                                                     00017190
   20 RETURN                                                            00017200
      END                                                               00017210
C                                                                       00017220
C                                                                       00017230
      SUBROUTINE ARGCHK(E,ESQ)                                          00017240
C                       SUBROUTINE ARGCHK (VERSION 82360), PART OF PEM. 00017250
C                                                                       00017260
C                                                                       00017270
C     SUBROUTINE ARGCHK LIMITS THE ARGUMENTS OF EXP(ESQ)*ERFC(E)        00017280
C     TO AVOID OVERFLOW/UNDERFLOW ERRORS.                               00017290
C                                                                       00017300
C                                                                       00017310
C     PEM ALGORITHMS AND PROGRAM DEVELOPMENT:  DECEMBER 1982            00017320
C     K. SHANKAR RAO                                                    00017330
C     NOAA-ATDL, P.O. BOX-E                                             00017340
C     OAK RIDGE, TENN 37830                                             00017350
C                                                                       00017360
C                                                                       00017370
      COMMON/EXPCHK/EXPMAX,EXPMIN,ETAMAX                                00017380
C                                                                       00017390
C                                                                       00017400
      ESQ=EXPMAX                                                        00017410
      IF(E.LT.0.) NSIGN=-1                                              00017420
      IF(E.GE.0.) NSIGN=1                                               00017430
      E=NSIGN*ETAMAX                                                    00017440
      RETURN                                                            00017450
      END                                                               00017460
C                                                                       00017470
C                                                                       00017480
      SUBROUTINE INMOD                                                  00017490
C                    SUBROUTINE INMOD  (VERSION 82360), PART OF PEM.    00017500
C                                                                       00017510
C                                                                       00017520
C  SUBROUTINE INMOD READS IN ALL INPUTS TO THE MODEL, SCREENS THEM,     00017530
C    PRINTS WARNING MESSAGES, AND INSERTS DEFAULT VALUES AS NEEDED.     00017540
C    THE SUBROUTINE PRINTS OUT LISTS OF THE CONTROL PARAMETERS,         00017550
C    SCENARIO PARAMETERS, AND SOURCE DATA FOR REFERENCE.                00017560
C    INMOD ALSO PROCESSES THE INPUT FOR EACH SCENARIO BEFORE            00017570
C    TRANSMITTING IT TO THE MAIN PROGRAM.                               00017580
C                                                                       00017590
C                                                                       00017600
C *** PEM MODIFICATIONS AND FORMATS BY M.M. STEVENS,                    00017610
C     NOAA-ATDL, P.O. BOX-E, OAK RIDGE, TENN 37830                      00017620
C     DECEMBER 1982                                                     00017630
C                                                                       00017640
C                                                                       00017650
      COMMON/PEMCOM/CONC(50,50,2),SDF(50,50,2),  TT(20),                00017660
```

```
     1 XP(300),YP(300),EP(300,2),HP(300),DP(300),VP(300),TP(300),       00017670
     2 XA(50),YA(50),EA(50,2),SIZE(50),                                 00017680
     3 WD(24),WS(24),TA(24),HMIX(24),PEN(24),                           00017690
     4 AX(7,3),BX(7,3),P(7),SCLAB(7),DTDZ(2),  SECTAN(16),              00017700
     5 XSWC,YSWC,GRID,LX,LY,    A(2),B(2),POLNAM(3,2),CALNAM(7,2),      00017710
     6 ITA,IRD,IWR,IDSK,        D80,D47,D8047,DIST,DELTA,               00017720
     7 ESH(2),PEAK,IBUOY,IRISE,IDWN,EFF,XS,    UINV,WVEC,               00017730
     8 NAS,NPS,INDEX,IGRID,IAV,ISCEN,IWDOPT,IWD,ISC,IPS,                00017740
     9 NTOPT,NWDOPT,NWSOPT,NSCEN,NLIST,NARRAY,NTAPE,NCSOPT,NMAX,        00017750
     * NSTDWN,INTER,NPRINT                                              00017760
C                                                                       00017770
      COMMON/CSWOR/NWORST(25,25,5),CWORST(25,25,5)                      00017780
      COMMON/PARM1/NPOL,ICT,VD1,W1,VD2,W2,TAUC                          00017790
      COMMON/PARM1A/GAMMA                                               00017800
C                                                                       00017810
      DIMENSION NAME(2),WDINC(6),SUMAQ(2),SUMPQ(2),SUMAR(2),EAR(2),     00017820
     1 AMSG(2),CWS(6)                                                   00017830
      DIMENSION DCR(24,2),NSC(24),NWD(24),NWS(24),ASCALE(2)             00017840
      DATA NAME/4H    ,4H    /                                          00017850
      DATA AMSG/4HVD1 ,4HVD2 /                                          00017860
      DATA WDINC/1.5707963,0.7853982,0.5235988,0.2617994,               00017870
     1           0.1745329,0.08726646/                                  00017880
      DATA CWS/1.5,2.46,4.47,6.93,9.61,12.52/                           00017890
C                                                                       00017900
      IF(INDEX.NE.0) GO TO 300                                          00017910
C                                                                       00017920
      ISTOP=0                                                           00017930
C                                                                       00017940
C  R E A D   A L L   I N P U T   D A T A .                              00017950
C                                                                       00017960
C **** READ FIRST CONTROL PARAMETER CARD (TITLE).                       00017970
C                                                                       00017980
      READ(IRD,800)TT                                                   00017990
      WRITE(IWR,900) TT                                                 00018000
C                                                                       00018010
C **** READ SECOND CONTROL PARAMETER CARD (OPTIONS).                    00018020
C                                                                       00018030
C     NTOPT  = AVERAGING TIME OPTION (1 OR 2 OR 3).                     00018040
C     NWDOPT = WIND DIRECTION INPUT OPTION (0 TO 7).                    00018050
C     NWSOPT = WIND SPEED INPUT OPTION (0 OR 1).                        00018060
C     NSCEN  = NUMBER OF SCENARIOS (1 TO 24).                           00018070
C     NLIST  = OUTPUT OPTION: LISTS OF CONC AND SURF DEP FLUX (0 OR 1)  00018080
C     NARRAY = OUTPUT OPTION: MAPS OF CONC AND SURF DEP FLUX (0 TO 3)   00018090
C     NTAPE  = OUTPUT OPTION: TAPE OF CONC AND SURF DEP FLUX (0 OR 1)   00018100
C     NCSOPT = OUTPUT OPTION: POINT SOURCE CULPABILITY LIST (0 OR 1).   00018110
C     NMAX   = OUTPUT OPTION: MAXIMUM CONC. FOR EACH SCENARIO (0 OR 1). 00018120
C     NSTDWN = STACK-TIP DOWNWASH OPTION (0 OR 1).                      00018130
C     INTER  = RECEPTOR INTERVAL ON TAPE OUTPUT (1,2,---).              00018140
C     NPRINT = OUTPUT OPTION: POINT SOURCE PLUME RISE INFO (0 OR 1)     00018150
C     INPTSC = INPUT OPTN: POINT SOURCE DATA ON UNIT IRD OR IDSK (1 OR 2)00018160
C                                                                       00018170
      READ(IRD,805)NTOPT,NWDOPT,NWSOPT,NSCEN,NLIST,NARRAY,NTAPE,        00018180
     1 NCSOPT,NMAX,NSTDWN,INTER,NPRINT,INPTSC                           00018190
C                                                                       00018200
      IF(NTOPT.GE.1 .AND. NTOPT.LE.3) GO TO 2                           00018210
      WRITE(IWR,660) NTOPT                                              00018220
      NTOPT=1                                                           00018230
    2 IF(NWDOPT.LE.1) GO TO 6                                           00018240
      IF(NWDOPT.GT.7) GO TO 5                                           00018250
      IF(NTOPT.EQ.1 .OR. NWDOPT.LE.1) GO TO 6                           00018260
      WRITE(IWR,615)                                                    00018270
    5 NWDOPT=0                                                          00018280
    6 IF(NWSOPT.GT.1) NWSOPT=0                                          00018290
      IF(NSCEN.EQ.0) NSCEN=1                                            00018300
      IF(NTOPT.EQ.2 .AND. NSCEN.NE.24) GO TO 500                        00018310
   10 IF(NSCEN.GT.24) GO TO 510                                         00018320
   20 IF(NLIST.EQ.0) GO TO 25                                           00018330
      IF(NLIST.GT.1) GO TO 22                                           00018340
      IF(NWDOPT.LE.1) GO TO 25                                          00018350
      WRITE(IWR,605)                                                    00018360
   22 NLIST=0                                                           00018370
   25 IF(NARRAY.GT.3) NARRAY=0                                          00018380
      IF(NTAPE.EQ.0) GO TO 40                                           00018390
      IF(NTAPE.GT.1) GO TO 30                                           00018400
      IF(NWDOPT.LE.1) GO TO 40                                          00018410
      WRITE(IWR,620)                                                    00018420
   30 NTAPE=0                                                           00018430
   40 IF(NCSOPT.GT.1) NCSOPT=0
      IF(NMAX.GT.1) NMAX=0
      IF(NSTDWN.GT.1) NSTDWN=0
      IF(INTER.EQ.0) INTER=1
      IF(NPRINT.GT.1) NPRINT=0
      IF(INPTSC.LT.1 .OR. INPTSC.GT.2) INPTSC=1
C
C      SET LABEL FOR TIME AVERAGING
      IAV=1
      IF(NTOPT.EQ.2) IAV=24
      IF (NTOPT.EQ.3) IAV=NSCEN
C
C  **** READ THIRD CONTROL PARAMETER CARD (GRID, DTDZ)
C
C    XRSWC,YRSWC = COORDINATES OF SOUTHWEST CORNER OF RECEPTOR GRID (KM)
C    LX          = NUMBER OF COLUMNS IN RECEPTOR GRID.
C    LY          = NUMBER OF ROWS IN RECEPTOR GRID.
C    GRID        = SPACING BETWEEN ROWS AND COLUMNS OF RECEPTOR GRID (KM)
C
C    DTDZ(1&2) = VERTICAL POTENTIAL TEMPERATURE GRADIENT
C                   FOR STABILITY CLASSES E & F.
C
      READ(IRD,810)XRSWC,YRSWC,LX,LY,GRID,DTDZ(1),DTDZ(2)
C
      IF(LX.EQ.0) LX=1
      IF(LY.EQ.0) LY=1
      IF(NTAPE.EQ.0) GO TO 115
C
      NRECS=((LX+1)/INTER)*((LY+1)/INTER)*NSCEN
      IF(NTOPT.EQ.2) NRECS= NRECS/24
      IF(NTOPT.EQ.3) NRECS= NRECS/NSCEN
      IF(NRECS.LT.10000) GO TO 115
      WRITE(IWR,600)
      NTAPE=0
  115 CONTINUE
C
C  **** READ FOURTH CONTROL PARAMETER CARD (POLLUTANTS)
C
C    NPOL  = NUMBER OF POLLUTANTS (1 OR 2)
C    ICT   = CHEMICAL TRANSFORMATION OR DECAY OPTION (0 OR 1)
C    VD1   = DEPOSITION VELOCITY FOR POLLUTANT SPECIES-1 (CM/S)
C    W1    = SETTLING VELOCITY FOR POLLUTANT SPOECIES-1 (CM/S)
C    VD2   = DEPOSITION VELOCITY FOR POLLUTANT SPECIES-2 (CM/S)
C    W2    = SETTLING VELOCITY FOR POLLUTANT SPECIES-2 (CM/S)
C    XKT   = CHEMICAL TRANSFORMATION OR DECAY RATE OF POLLUTANT
C              SPECIES-1 (PERCENT PER HOUR)
C    GAMMA = RATIO OF MOLECULAR WEIGHTS OF SPECIES-2 (PRODUCT)
C              TO SPECIES-1 (REACTANT) IN CHEMICAL TRANSFORMATION
C
C  NOTE: FOR DEPOSITION TO OCCUR, W SHOULD BE LESS THAN OR EQUAL TO VD.
C        FOR DEPOSITION OF GASES AND VERY SMALL PARTICLES, W=0.
C        FOR DEPOSITION OF SMALL PARTICLES, W IS LESS THAN VD.
C        FOR DEPOSITION OF MEDIUM AND LARGE PARTICLES, W=VD.
C
      READ (IRD,812) NPOL,ICT,VD1,W1,VD2,W2,XKT,GAMMA
C
      IF(NPOL.LT.1 .OR. NPOL.GT.2) NPOL=1
      IF(NPOL.EQ.1 .OR. NCSOPT.EQ.0) GO TO 116
      WRITE(IWR,635)
      NCSOPT=0
  116 IF(W1.GT.VD1) W1=VD1
      IF(NPOL.EQ.2) GO TO 117
      VD2=0.0
      W2=0.0
      GO TO 118
  117 IF(W2.GT.VD2) W2=VD2
  118 IF(ICT.EQ.1) GO TO 119
      XKT=0.0
      GAMMA=0.0
      GO TO 122
  119 IF(XKT.GE.0.1 .AND. XKT.LE.100.) GO TO 120
      TXKT=0.1
      IF(XKT.GT.100.) TXKT=100.
      WRITE(IWR,640) XKT,TXKT
      XKT=TXKT
C
C    CONVERT CHEMICAL TRANSFORMATION RATE XKT (PERCENT PER HOUR) TO
```

```
C     THE EQUIVALENT TIME SCALE TAUC (SECONDS).
  120 TAUC=0.36E06/XKT
C
  122 IF(NCSOPT.EQ.0 .OR. (LX.LE.25 .AND. LY.LE.25)) GO TO 125
      WRITE(IWR,645)
      NCSOPT=0
C
C     SHIFT THE RECEPTOR GRID TO THE COMPUTATION GRID.
125   XSWC= XRSWC - 0.5*GRID
      YSWC= YRSWC - 0.5*GRID
C
130   IF(DTDZ(1).LT.0.00001) DTDZ(1)=0.020
      IF(DTDZ(2).LT.0.00001) DTDZ(2)=0.035
C
C  IF GRID IS ZERO, SWITCH ON AUTOMATIC GRID OPTION.
      IGRID=0
      IF(GRID.LT.1.0E-5) IGRID=1
      IF(IGRID.EQ.1.AND.NTOPT.GT.1) GO TO 520
C
C **** READ 5TH CONTROL PARAMETER CARD (AREA SOURCE SCALING,CALIBRATION)
C
C    ASCALE(1&2) = AREA SOURCE EMISSION SCALING FACTORS
C                    FOR EACH POLLUTANT.
C    A(1&2)      = CONCENTRATION CALIBRATION FACTOR (INTERCEPT)
C                    FOR EACH POLLUTANT.
C    B(1&2)      = CONCENTRATION CALIBRATION FACTOR (SLOPE)
C                    FOR EACH POLLUTANT.
C
  135 READ(IRD,815) ASCALE,A(1),B(1),A(2),B(2)
C
      IF(ASCALE(1).LE.0.) ASCALE(1)=1.0
      IF(ASCALE(2).LE.0.) ASCALE(2)=1.0
C
C  **** READ CARD 6 (POLLUTANT AND CALIBRATION LABELS)
C
      READ(IRD,817)(POLNAM(I,1),I=1,3),(CALNAM(I,1),I=1,7),
     1             (POLNAM(I,2),I=1,3),(CALNAM(I,2),I=1,7)
C
C  **** READ ONE TO 24 SCENARIO PARAMETER CARDS.
C
C     NSC       = STABILITY CLASS NUMBER (1 TO 7)
C     NWS       = WIND SPEED CLASS NUMBER (1 TO 6)
C     NWD       = WIND SECTOR NUMBER (1 TO 16)
C     WS        = WIND SPEED (M/S)
C     WD        = WIND DIRECTION (DEGREES)
C     TA        = AMBIENT TEMPERATURE (DEGREES CELSIUS)
C     PEN       = INVERSION PENETRATION FACTOR (PEN .GE. 1.0)
C     HMIX      = MIXING HEIGHT (METERS)
C
      DO 150 IS=1,NSCEN
      READ(IRD,820)NSC(IS),NWS(IS),NWD(IS),WS(IS),WD(IS),TA(IS),
     1 PEN(IS),HMIX(IS)
C
      IF(NSC(IS).GE.1 .AND. NSC(IS).LE.7) GO TO 140
      NUM=1
      IF(NSC(IS).GT.7) NUM=7
      WRITE(IWR,535) IS,NSC(IS),NUM
      NSC(IS)=NUM
  140 IF(NWSOPT.EQ.0) GO TO 142
      IF(NWS(IS).GE.1 .AND. NWS(IS).LE.6) GO TO 144
      NUM=1
      IF(NWS(IS).GT.6) NUM=6
      WRITE(IWR,545) IS,NWS(IS),NUM
      NWS(IS)=NUM
      GO TO 144
  142 IF(WS(IS).GT.0.) GO TO 144
      WRITE(IWR,565) IS,WS(IS)
      WS(IS)=1.0
  144 IF(NWDOPT.NE.1) GO TO 146
      IF(NWD(IS).GE.1 .AND. NWD(IS).LE.16) GO TO 146
      NUM=1
      IF(NWD(IS).GT.16) NUM=16
      WRITE(IWR,555) IS,NWD(IS),NUM
      NWD(IS)=NUM
  146 IF(PEN(IS).LT.1.0) PEN(IS)=2.0
      IF(HMIX(IS).LT.1.0E-5) HMIX(IS)= 9999.9
  150 CONTINUE
```

```
C
C  PRINT INPUT CONTROL PARAMETERS
C
      IF(ISTOP.EQ.1) WRITE(IWR,900) TT
      WRITE(IWR,902) NTOPT
      WRITE(IWR,904) NWDOPT
      WRITE(IWR,906) NWSOPT
      WRITE(IWR,908) NSCEN
      WRITE(IWR,910) NSTDWN
      IF(IGRID.EQ.0) WRITE(IWR,916) LX,LY,GRID,XRSWC,YRSWC
      IF(IGRID.EQ.1) WRITE(IWR,914)
      WRITE(IWR,920) DTDZ(1),DTDZ(2)
      WRITE(IWR,900) TT
      WRITE(IWR,922) NPOL,(POLNAM(I,1),I=1,3)
      IF(NPOL.EQ.2) WRITE(IWR,923) (POLNAM(I,2),I=1,3)
      WRITE(IWR,924) ASCALE(1)
      IF(NPOL.EQ.2) WRITE(IWR,935) ASCALE(2)
      WRITE(IWR,925) A(1),B(1)
      IF(NPOL.EQ.2) WRITE(IWR,926) A(2),B(2)
      WRITE(IWR,927) (CALNAM(I,1),I=1,7)
      IF(NPOL.EQ.2) WRITE(IWR,921) (CALNAM(I,2),I=1,7)
      WRITE(IWR,928) VD1
      IF(NPOL.EQ.2) WRITE(IWR,931) VD2
      WRITE(IWR,929) W1
      IF(NPOL.EQ.2) WRITE(IWR,933) W2
      WRITE(IWR,930) ICT
      IF(NPOL.EQ.1) WRITE(IWR,932)
      IF(NPOL.EQ.2) WRITE(IWR,934)
      IF(ICT.EQ.0) GO TO 152
      WRITE(IWR,936) XKT
      WRITE(IWR,938) GAMMA
  152 WRITE(IWR,940)
      IF(NLIST.GT.0) WRITE(IWR,942) NLIST
      IF(NARRAY.GT.0) WRITE(IWR,944) NARRAY
      IF(NARRAY.EQ.1) WRITE(IWR,946)
      IF(NARRAY.EQ.2) WRITE(IWR,948)
      IF(NARRAY.EQ.3) WRITE(IWR,950)
      IF(NTAPE.GT.0) WRITE(IWR,952) NTAPE,INTER
      IF(NCSOPT.GT.0) WRITE(IWR,954) NCSOPT
      IF(NPRINT.GT.0) WRITE(IWR,956) NPRINT
      IF(NMAX.GT.0) WRITE(IWR,958) NMAX
C
C     PRINT INPUT PARAMETERS FOR SCENARIOS
C
      WRITE(IWR,960)TT
      WRITE(IWR,962)
      WRITE(IWR,963)
      WRITE(IWR,964)
C
      DO 160 IS=1,NSCEN
      KS=NSC(IS)
      WRITE(IWR,966) IS,SCLAB(KS)
      IF(NWSOPT.EQ.0) GO TO 153
      KW=NWS(IS)
      WS(IS)=CWS(KW)
      WRITE(IWR,970) KW
  153 WRITE(IWR,972) WS(IS)
      IF(NWDOPT.EQ.1) GO TO 155
      WDOUT=WD(IS)
      GO TO 156
  155 KD=NWD(IS)
      WDOUT=SECTAN(KD) * 180./3.14159265
      WRITE(IWR,974) KD
  156 WRITE(IWR,978) WDOUT,TA(IS),PEN(IS),HMIX(IS)
      WD(IS)= WD(IS)*3.14159265/180.
      TA(IS)= TA(IS) + 273.15
C
C  FOR EACH SCENARIO, CALCULATE THE CRITICAL DOWNWIND DISTANCES
C    AT WHICH VERTICAL MIXING IMPENDS (DCRIT(IS,1)) AND IS COMPLETE
C    (DCRIT(IS,2)).
      JSC=NSC(IS)
      JD=3
      IF(AX(JSC,2)*5000.**BX(JSC,2).GT.0.47*HMIX(IS)) JD=2
      IF(AX(JSC,1)*500.**BX(JSC,1).GT.0.47*HMIX(IS))  JD=1
      DCR(IS,1)=0.001*(0.47*HMIX(IS)/AX(JSC,JD))**(1./BX(JSC,JD))
      DCR(IS,2)= DCR(IS,1)*2.
 160  CONTINUE
```

```
C
C  **** READ UP TO 50 AREA SOURCE CARDS.
C
C    XA,YA   = COORDINATES OF SOUTHWEST CORNER OF AREA SOURCE (KM).
C    SIZE    = LENGTH OF A SIDE OF AREA SOURCE (M).
C    EA(1&2) = EMISSION RATES OF 2 POLLUTANTS (G/S).
C
      WRITE(IWR,990) TT
      NAS=1
      SUMAQ(1)=0.
      SUMAQ(2)=0.
      SUMAR(1)=0.
      SUMAR(2)=0.
C
170   READ(IRD,825)XA(NAS),YA(NAS),SIZE(NAS),EA(NAS,1),EA(NAS,2)
C
      IF(NPOL.EQ.1) EA(NAS,2)=0.0
      IF((SIZE(NAS)+EA(NAS,1)+EA(NAS,2)).LT.1.0E-04) GO TO 180
      IF(SIZE(NAS).GE.1.0E-4) GO TO 172
      SIZE(NAS)=1.0E-4
      IF(GRID.NE.0.) SIZE(NAS)=GRID*1000.
      WRITE(IWR,585) NAS,SIZE(NAS)
  172 DO 175 K=1,2
      EAR(K)=EA(NAS,K)
      SUMAR(K)=SUMAR(K)+EAR(K)
      EA(NAS,K)= EA(NAS,K)*ASCALE(K)
175   SUMAQ(K)=SUMAQ(K)+EA(NAS,K)
C
C   PRINT INPUT PARAMETERS FOR THIS AREA SOURCE
      WRITE(IWR,992)NAS,XA(NAS),YA(NAS),SIZE(NAS),EAR(1),EA(NAS,1),
     1EAR(2),EA(NAS,2)
C
      SIZE(NAS)=SIZE(NAS)*0.001
      IF(NAS/50*50.EQ.NAS) WRITE(IWR,990)TT
      NAS=NAS+1
      GO TO 170
180   NAS=NAS-1
      WRITE(IWR,994) SUMAR(1),SUMAQ(1),SUMAR(2),SUMAQ(2)
C
C   IF AREA SOURCE CALCULATIONS ARE TO BE MADE, THEN DEPOSITION VELOCITY
C    VALUE(S) MUST BE GREATER THAN ZERO
      IF(NAS.LT.1) GO TO 184
      IF(VD1.GT.0.) GO TO 181
      WRITE(IWR,655) AMSG(1)
      VD1=0.01
  181 IF(NPOL.EQ.1 .OR. VD2.GT.0.) GO TO 184
      WRITE(IWR,655) AMSG(2)
      VD2=0.01
C
C
C  **** READ UP TO 300 POINT SOURCES
C
C    XP,YP   = COORDINATES OF POINT SOURCE (KM).
C    EP(1&2) = EMISSION RATES OF 2 POLLUTANTS (G/S).
C    HP      = SOURCE HEIGHT (M).
C    DP      = INSIDE DIAMETER (M).
C    VP      = VELOCITY (M/S).
C    TP      = TEMPERATURE (DEGREES CELSIUS).
C    NAME    = IDENTIFICATION.
C
  184 WRITE(IWR,980) TT
      NPS=1
      SUMPQ(1)=0.
      SUMPQ(2)=0.
C
  185 IF(INPTSC.EQ.2)READ(IDSK,830)XP(NPS),YP(NPS),EP(NPS,1),EP(NPS,2),
     1 HP(NPS),DP(NPS),VP(NPS),TP(NPS),NAME(1),NAME(2)
      IF(INPTSC.EQ.1) READ(IRD,830)XP(NPS),YP(NPS),EP(NPS,1),EP(NPS,2),
     1 HP(NPS),DP(NPS),VP(NPS),TP(NPS),NAME(1),NAME(2)
C
      IF(NPOL.EQ.1) EP(NPS,2)=0.0
      IF(HP(NPS)+DP(NPS)+VP(NPS)+TP(NPS).LT.1.0E-4) GO TO 190
      IF(DP(NPS).GT.0.0) GO TO 187
      WRITE(IWR,575) NPS
      DP(NPS)=1.0E-4
C
C  PRINT INPUT PARAMETERS FOR THIS POINT SOURCE
```

```
  187 WRITE(IWR,984) NPS,NAME(1),NAME(2),XP(NPS),YP(NPS),EP(NPS,1),     00021520
     1 EP(NPS,2),HP(NPS),DP(NPS),VP(NPS),TP(NPS)                        00021530
C                                                                       00021540
      TP(NPS)=TP(NPS)+273.15                                            00021550
      IF(NPS/50*50.EQ.NPS) WRITE(IWR,980)TT                             00021560
      SUMPQ(1)=SUMPQ(1)+EP(NPS,1)                                       00021570
      SUMPQ(2)=SUMPQ(2)+EP(NPS,2)                                       00021580
      NPS=NPS+1                                                         00021590
      GO TO 185                                                         00021600
190   NPS= NPS-1                                                        00021610
      WRITE(IWR,986) SUMPQ(1),SUMPQ(2)                                  00021620
C                                                                       00021630
C    IF THERE WERE SERIOUS ERRORS IN INPUT PARAMETERS, STOP             00021640
      IF(ISTOP.EQ.0) GO TO 195                                          00021650
      WRITE(IWR,630)                                                    00021660
      STOP                                                              00021670
C                                                                       00021680
C   INITIALIZE FOR FIRST CALL TO INMOD FOR SCENARIO PREPARATION         00021690
  195 IWDOPT= 0                                                         00021700
      ISCEN=0                                                           00021710
      RETURN                                                            00021720
C                                                                       00021730
C                                                                       00021740
C  P R E P A R E   S C E N A R I O   I N F O R M A T I O N .            00021750
C                                                                       00021760
300   IF(NWDOPT.LE.1) GO TO 350                                         00021770
      IF(ISCEN.EQ.0.OR.IWDOPT.GE.4) GO TO 320                           00021780
      IWDOPT= IWDOPT + 1                                                00021790
      WD(ISCEN)= WD(ISCEN) + WDINC(NWDOPT-1)                            00021800
      IF(WD(ISCEN).GE.6.2831853) WD(ISCEN)=WD(ISCEN) - 6.2831853        00021810
      GO TO 353                                                         00021820
320   ISCEN= ISCEN + 1                                                  00021830
      IWDOPT= 1                                                         00021840
      GO TO 353                                                         00021850
350   ISCEN= ISCEN + 1                                                  00021860
353   ISC=NSC(ISCEN)                                                    00021870
      IWD=NWD(ISCEN)                                                    00021880
      D47= DCR(ISCEN,1)                                                 00021890
      D80= DCR(ISCEN,2)                                                 00021900
      D8047= D80 - D47                                                  00021910
      IF(NCSOPT.EQ.0) GO TO 400                                         00021920
      DO 380 I=1,25                                                     00021930
      DO 380 J=1,25                                                     00021940
      DO 380 K=1,5                                                      00021950
      NWORST(I,J,K)=0                                                   00021960
380   CWORST(I,J,K)=0.                                                  00021970
400   RETURN                                                            00021980
C                                                                       00021990
C   ERROR MESSAGES                                                      00022000
C                                                                       00022010
  500 WRITE(IWR,505)                                                    00022020
  505 FORMAT(1H0,'WHEN TIME AVG OPTION NTOPT=2, NUMBER OF SCENARIOS MUST00022030
     1 =24')                                                            00022040
      ISTOP=1                                                           00022050
      GO TO 10                                                          00022060
  510 WRITE(IWR,515) NSCEN                                              00022070
  515 FORMAT(1H0,'MAXIMUM NUMBER OF SCENARIOS ALLOWED IS 24. NSCEN=',I4)00022080
      ISTOP=1                                                           00022090
      GO TO 20                                                          00022100
  520 WRITE(IWR,525)                                                    00022110
  525 FORMAT(1H0,'AUTOGRID MAY NOT BE USED WITH TIME AVG OPTION NTOPT>1'00022120
     1)                                                                 00022130
      ISTOP=1                                                           00022140
      GO TO 135                                                         00022150
  535 FORMAT(1H0,'IN SCENARIO',I3,' STABILITY CLASS NUMBER NSC=',I2,    00022160
     1' IS OUT OF RANGE.  NSC SET TO',I2)                               00022170
  545 FORMAT(1H0,'IN SCENARIO',I3,' WIND SPEED CLASS NUMBER NWS=',I2,   00022180
     1' IS OUT OF RANGE.  NWS SET TO',I2)                               00022190
  555 FORMAT(1H0,'IN SCENARIO',I3,' WIND DIRECTION SECTOR NUMBER NWD=', 00022200
     1 I3,' IS OUT OF RANGE.  NWD SET TO',I3)                           00022210
  565 FORMAT(1H0,'IN SCENARIO',I3,' SPECIFIED WIND SPEED MUST BE GREATER00022220
     1 THAN ZERO.  WS SET TO 1.0 M/S')                                  00022230
  575 FORMAT(1H0,'POINT SOURCE',I4,':  INSIDE DIAMETER MUST BE GREATER T00022240
     1HAN ZERO.  DP SET TO .0001 M')                                    00022250
  585 FORMAT(1H0,'AREA SOURCE',I3,':  LENGTH OF SIDE MUST BE GREATER THA00022260
     1N ZERO.  SIZE SET TO ',F9.2)                                      00022270
600   FORMAT(1H0,'RUN REQUESTED WOULD PRODUCE OVER 10000 RECORDS ON TAPE00022280
     1'/' OUTPUT OPTION NTAPE HAS BEEN SET TO ZERO')
 605 FORMAT(1H0,'OUTPUT OPTION NLIST MAY NOT BE USED WITH AUTOMATIC WIN
     1D SHIFT OPTION (NWDOPT>1)'/' NLIST HAS BEEN SET TO ZERO')
 615 FORMAT(1H0,'AUTOMATIC WIND SHIFT OPTION (NWDOPT>1) MAY NOT BE USED
     1 WITH TIME AVG OPTION NTOPT>1'/' NWDOPT HAS BEEN SET TO ZERO')
 620 FORMAT(1H0,'OUTPUT OPTION NTAPE MAY NOT BE USED WITH AUTOMATIC WIN
     1D SHIFT OPTION (NWDOPT>1)'/' NTAPE HAS BEEN SET TO ZERO')
 630 FORMAT(1H1//' SERIOUS ERROR(S) IN INPUT PARAMETERS',5X,
     1 'RUN CANNOT BE CONTINUED')
 635 FORMAT(1H0,'CONTROL STRATEGY OUTPUT OPTION NCSOPT MAY NOT BE USED
     1WITH TWO POLLUTANTS'/' NCSOPT HAS BEEN SET TO ZERO')
 640 FORMAT(1H0,'CHEMICAL TRANSFORMATION RATE XKT=',F7.3,' IS OUT OF RA
     1NGE'/' XKT HAS BEEN SET TO',F8.3)
 645 FORMAT(1H0,'CONTROL STRATEGY OUTPUT OPTION NCSOPT MAY NOT BE USED
     1WHEN NUMBER OF COLUMNS OR ROWS IN RECEPTOR GRID IS GREATER THAN 25
     2'/' NCSOPT HAS BEEN SET TO ZERO')
 655 FORMAT(1H0,'AREA SOURCE CALCULATIONS REQUIRE DEPOSITION VELOCITY G
     1REATER THAN ZERO.',4X,A4,'HAS BEEN SET TO 0.01')
 660 FORMAT(1H0,'TIME AVERAGING OPTION NTOPT=',I2,' IS OUT OF RANGE.  N
     1TOPT SET TO 1')
C
C   INPUT FORMATS
C
800   FORMAT(20A4)
805   FORMAT(13I5)
810   FORMAT(2F10.0,2I10,3F10.0)
812   FORMAT(2I5,6F10.0)
815   FORMAT(6F10.0)
817   FORMAT(3A4,7A4,3A4,7A4)
820   FORMAT(3I5,5F10.0)
825   FORMAT(5F10.0)
830   FORMAT(8F9.0,2A4)
C
C   OUTPUT FORMATS
C
 900 FORMAT(1H1,45X,'POLLUTION EPISODIC MODEL'///4X,'INPUT CONTROL PARA
     1METERS:  ',20A4//)
 902 FORMAT(10X,'AVERAGING TIME OPTION: NTOPT=',I1//
     1 18X,'A SCENARIO IS A SET OF METEOROLOGICAL DATA FOR ONE HOUR'//
     2 13X,'1  1 HOUR: CONCENTRATIONS ARE CALCULATED FOR EACH SCENARIO'/
     3 13X,'2  24 HOURS: CONCENTRATIONS CALCULATED FOR 24 SCENARIOS ARE
     4AVERAGED'/13X,'3  VARIABLE: CONCENTRATIONS CALCULATED FOR A GIVEN
     5NUMBER (2 TO 24) OF SCENARIOS ARE AVERAGED'//)
 904 FORMAT(10X,'WIND DIRECTION OPTION: NWDOPT=',I1//
     113X,'0  DIRECTION IN DEGREES TO BE SPECIFIED FOR EACH SCENARIO'/
     213X,'1  SECTOR NUMBER TO BE SPECIFIED FOR EACH SCENARIO'/
     312X,'2-7 DIRECTION IN DEGREES TO BE SPECIFIED FOR THE FIRST OF FOU
     4R SUB-SCENARIOS.'/17X,'FOR EACH SUCCEEDING SUB-SCENARIO, WIND DIRE
     5CTION IS AUTOMATICALLY INCREASED'/17X,'BY 90,45,30,15,10,OR 5 DEGR
     6EES, DEPENDING ON THE OPTION NUMBER SELECTED.'//)
 906 FORMAT(10X,'WIND SPEED OPTION: NWSOPT=',I1//
     113X,'0  SPEED IN M/S TO BE SPECIFIED FOR EACH SCENARIO'/
     213X,'1  WIND SPEED CLASS NUMBER TO BE SPECIFIED FOR EACH SCENARIO'
     3//)
 908 FORMAT(10X,'NUMBER OF SCENARIOS: NSCEN=',I2//)
 910 FORMAT(10X,'STACK-TIP DOWNWASH ALGORITHM OPTION: NSTDWN=',I1//
     1 13X,'0  ALGORITHM IS IN EFFECT'/
     2 13X,'1  ALGORITHM IS NOT USED'//)
 914 FORMAT(10X,'AUTOMATIC RECEPTOR GRID OPTION IS IN EFFECT'//)
 916 FORMAT(10X,'RECEPTOR GRID:',
     16X,'COLUMNS: LX=',I3,4X,'ROWS: LY=',I3/
     230X,'SPACING: GRID=',F7.3,' KM'/
     330X,'SOUTHWEST CORNER    XRSWC= ',F8.3,' KM W'/
     450X,'YRSWC= ',F8.3,' KM S'//)
 920 FORMAT(10X,'POTENTIAL TEMPERATURE GRADIENT: DTDZ(1)= ',F7.3,
     1' DEG/M    STABILITY CLASS E'/
     242X,'DTDZ(2)= ',F7.3,' DEG/M    STABILITY CLASS F'//)
 921 FORMAT(1H+,85X,7A4)
 922 FORMAT(10X,'NUMBER OF POLLUTANTS: NPOL=',I1/
     1 51X,'POLLUTANT-1: ',3A4)
 923 FORMAT(1H+,85X,'POLLUTANT-2: ',3A4)
 924 FORMAT(/10X,'AREA SOURCE SCALING FACTOR:',17X,'ASCALE=',F9.3)
 925 FORMAT(10X,'CALIBRATION COEFFICIENTS:',
     1 16X,'A=',F10.3,'  B=',F10.3)
 926 FORMAT(1H+,85X,'A=',F10.3,'  B=',F10.3)
 927 FORMAT(10X,'CALIBRATION IDENTIFICATION:',14X,7A4,6X,7A4)
 928 FORMAT(10X,'DEPOSITION VELOCITY (CM/S):',20X,'VD1=',F8.3)
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  929 FORMAT(10X,'SETTLING VELOCITY (CM/S):',23X,'W1=',F8.3)              00023060
  930 FORMAT(//10X,'CHEMICAL TRANSFORMATION OPTION: ICT=',I1/)            00023070
  931 FORMAT(1H+,91X,'VD2=',F8.3)                                         00023080
  932 FORMAT(13X,'NPOL=1'/                                                00023090
     215X,'ICT=0  CHEMICAL TRANSFORMATION LOSS OF POLLUTANT IS IGNORED'/00023100
     315X,'ICT=1  FIRST-ORDER CHEMICAL TRANSFORMATION LOSS OF POLLUTANT 00023110
     4IS CONSIDERED'//)                                                 00023120
  933 FORMAT(1H+,92X,'W2=',F8.3)                                          00023130
  934 FORMAT(13X,'NPOL=2'/                                                00023140
     215X,'ICT=0  CHEMICAL TRANSFORMATION LOSS OF POLLUTANTS IS IGNORED'00023150
     3/15X,'ICT=1  FIRST-ORDER CHEMICAL TRANSFORMATION OF POLLUTANT-1 TO00023160
     4 POLLUTANT-2 IS CONSIDERED'//)                                    00023170
  935 FORMAT(1H+,88X,'ASCALE=',F9.3)                                      00023180
  936 FORMAT(10X,'CHEMICAL TRANSFORMATION RATE: XKT=',F7.3,               00023190
     1' PERCENT/HR'/)                                                   00023200
  938 FORMAT(10X,'RATIO OF MOLECULAR WEIGHTS OF POLLUTANT-2 (PRODUCT) TO00023210
     1 POLLUTANT-1 (REACTANT): GAMMA=',F6.3/)                           00023220
  940 FORMAT(//9X,'OUTPUT OPTIONS SELECTED:'/)                            00023230
  942 FORMAT(13X,'NLIST=',I1,3X,'LISTS OF CONCENTRATION AND SURFACE DEPO00023240
     1SITION FLUX AT EACH RECEPTOR IN THE GRID,'/24X,'ONE COLUMN PER PAG00023250
     2E')                                                               00023260
  944 FORMAT(13X,'NARRAY=',I1,2X,'MAPS OF CONCENTRATION AND SURFACE DEPO00023270
     1SITION FLUX AT EACH RECEPTOR IN THE GRID,')                       00023280
  946 FORMAT(24X,'CALIBRATED AND UNCALIBRATED')                           00023290
  948 FORMAT(24X,'UNCALIBRATED ONLY')                                     00023300
  950 FORMAT(24X,'CALIBRATED ONLY')                                       00023310
  952 FORMAT(13X,'NTAPE=',I1,3X,'TAPE CONTAINING COORDINATES, CONCENTRAT00023320
     1ION, AND SURFACE DEPOSITION FLUX'/24X,'AT EACH RECEPTOR IN THE GRI00023330
     2D'/13X,'INTER=',I2,2X,'INTERVAL OF RECEPTORS WHICH WILL BE WRITTEN00023340
     3 ON TAPE')                                                        00023350
  954 FORMAT(13X,'NCSOPT=',I1,2X,'LIST OF POINT SOURCE CULPABILITY FOR C00023360
     1ONCENTRATION AND SURFACE DEPOSITION FLUX'/24X,'AT EACH RECEPTOR IN00023370
     2 THE GRID')                                                       00023380
  956 FORMAT(13X,'NPRINT=',I1,2X,'LIST OF POINT SOURCE PARAMETERS AND EF00023390
     1FECTIVE STACK HEIGHTS'/24X,'PRINTED AT BEGINNING OF EACH SCENARIO'00023400
     2)                                                                 00023410
  958 FORMAT(13X,'NMAX=',I1,4X,'LIST OF RECEPTORS WITH HIGHEST CONCENTRA00023420
     1TION AND SURFACE DEPOSITION FLUX'/24X,'FOR EACH SCENARIO - PRINTED00023430
     2 AT END OF RUN')                                                  00023440
  960 FORMAT(1H1,45X,'POLLUTION EPISODIC MODEL'///4X,'INPUT SCENARIO PAR00023450
     1AMETERS:  ',20A4//26X,'WIND DIRECTIONS',27X,'WIND SPEED CLASSES', 00023460
     212X,'STABILITY CLASSES'/)                                         00023470
  962 FORMAT(10X,'SECTOR    DIRECTION',6X,'SECTOR    DIRECTION',9X,     00023480
     1'CLASS   SPEED    CLASS',15X,'CLASS'/                             00023490
     210X,'NUMBER',8X,'(DEG)',6X,'NUMBER',8X,'(DEG)',9X,'INDEX   (M/S)  00023500
     3 INTERVAL(KT)',9X,'INDEX   CLASS'//13X,'1    N',7X,'0.0',9X,'9    00023510
     4S',5X,'180.0'/13X,'2    NNE    22.5',8X,'10    SSW   202.5',11X,  00023520
     5'1',6X,'1.50',7X,'0-3',16X,'1',7X,'A'/13X,'3    NE',5X,'45.0',8X, 00023530
     6'11    SW    225.0',11X,'2',6X,'2.46',7X,'4-6',16X,'2',7X,'B')    00023540
  963 FORMAT(13X,'4    ENE    67.5',8X,'12    WSW   247.5',11X,'3',6X,  00023550
     1'4.47',7X,'7-10',15X,'3',7X,'C'/13X,'5    E',6X,'90.0',8X,'13    W00023560
     2',5X,'270.0',11X,'4',6X,'6.93',6X,'11-16',15X,'4',7X,'DD (DAY)'/  00023570
     313X,'6    ESE   112.5',8X,'14    WNW   292.5',11X,'5',6X,'9.61',  00023580
     46X,'17-21',15X,'5',7X,'DN (NIGHT)'/13X,'7    SE    135.0',8X,'15  00023590
     5 NW    315.0',11X,'6',5X,'12.52    OVER 21',15X,'6',7X,'E'/       00023600
     613X,'8    SSE   157.5',8X,'16    NNW   337.5',48X,'7',7X,'F'///)  00023610
  964 FORMAT(5X,'SCENARIO',3X,'STABILITY',3X,'WIND SPEED',5X,'WIND',8X, 00023620
     1'WIND',6X,'WIND',8X,'AMBIENT',9X,'INVERSION',8X,'MIXING'/         00023630
     26X,'NUMBER',6X,'CLASS',7X,'CLASS',8X,'SPEED',6X,'SECTOR',3X,      00023640
     3'DIRECTION',3X,'TEMPERATURE',3X,'PENETRATION FACTOR',3X,'HEIGHT'/ 00023650
     443X,'(M/S)',17X,'(DEG)',7X,'(DEG C)',27X,'(M)'/)                  00023660
  966 FORMAT(8X,I2,10X,A2)                                                00023670
  970 FORMAT(1H+,31X,I1)                                                  00023680
  972 FORMAT(1H+,42X,F6.3)                                                00023690
  974 FORMAT(1H+,55X,I2)                                                  00023700
  978 FORMAT(1H+,63X,F6.2,7X,F7.2,11X,F6.3,8X,F7.1)                       00023710
  980 FORMAT(1H1,45X,'POLLUTION EPISODIC MODEL'///4X,'INPUT POINT SOURCE00023720
     1 PARAMETERS:  ',20A4///                                           00023730
     26X,'POINT SOURCE',10X,'COORDINATES',9X,'EMISSION RATE',           00023740
     36X,'EMISSION RATE',5X,'HEIGHT',4X,'DIAMETER',4X,'EXIT VEL',5X,    00023750
     4'EXIT TEMP'/5X,'NUMBER',3X,'LABEL',7X,'X(KM)',5X,'Y(KM)',6X,      00023760
     5'POLLUTANT-1 (G/S)',2X,'POLLUTANT-2 (G/S)',3X,'(M)',8X,'(M)',8X,  00023770
     6'(M/S)',8X,'(DEG C)'/)                                            00023780
  984 FORMAT(6X,I3,3X,2A4,3X,F8.2,2X,F8.2,10X,F9.3,10X,F9.3,6X,F6.2,5X, 00023790
     1F6.3,6X,F7.3,6X,F8.3)                                             00023800
  986 FORMAT(1H0,5X,'SUMS OF THE POINT SOURCE EMISSION RATES',6X,F9.3,  00023810
     1' G/S',6X,F9.3,' G/S')                                            00023820
  990 FORMAT(1H1,45X,'POLLUTION EPISODIC MODEL'///4X,'INPUT AREA SOURCE 00023830
     1PARAMETERS:  ',20A4///                                            00023840
     270X,'POLLUTANT-1',17X,'POLLUTANT-2'/5X,'AREA SOURCE',8X,          00023850
     3'COORDINATES',9X,'LENGTH OF SIDE',11X,'EMISSION RATE',15X,        00023860
     4'EMISSION RATE'/                                                  00023870
     57X,'NUMBER',9X,'X(KM)',5X,'Y(KM)',13X,'(M)',12X,'INPUT (G/S)',    00023880
     64X,'SCALED',7X,'INPUT (G/S)',4X,'SCALED'/)                        00023890
  992 FORMAT(9X,I2,8X,F8.2,2X,F8.2,10X,F8.2,9X,F9.3,4X,F9.3,6X,         00023900
     1 F9.3,4X,F9.3)                                                    00023910
  994 FORMAT(1H0,5X,'SUMS OF THE AREA SOURCE EMISSION RATES IN THIS RUN'00023920
     1,8X,F9.3,4X,F9.3,6X,F9.3,4X,F9.3)                                 00023930
      END                                                               00023940
C                                                                       00023950
C                                                                       00023960
      SUBROUTINE OUTMOD                                                 00023970
C                    SUBROUTINE OUTMOD (VERSION 82360), PART OF PEM.    00023980
C                                                                       00023990
C                                                                       00024000
C     SUBROUTINE OUTMOD COORDINATES OUTPUT OF THE CONCENTRATION(S)      00024010
C     AND SURFACE DEPOSITION FLUX(ES) CALCULATED FOR EACH RECEPTOR      00024020
C     IN THE GRID FOR EACH SCENARIO.                                    00024030
C     ON OPTION, THE OUTPUT MAY BE IN THE FORM OF LISTS, ARRAY          00024040
C     MAPS, OR TAPE.                                                    00024050
C     OUTMOD CALLS SUBROUTINE SCENMX TO DETERMINE AND STORE THE         00024060
C     RECEPTORS WITH MAXIMUM CONCENTRATION(S) AND SURFACE DEPOSITION    00024070
C     FLUX(ES) FOR THE SCENARIO.                                        00024080
C                                                                       00024090
C                                                                       00024100
C *** PEM MODIFICATIONS AND FORMATS BY MARTHA M. STEVENS,               00024110
C     NOAA-ATDL, P.O. BOX-E, OAK RIDGE, TENN 37830                      00024120
C     DECEMBER 1982                                                     00024130
C                                                                       00024140
C                                                                       00024150
      COMMON/PEMCOM/CONC(50,50,2),SDF(50,50,2),  TT(20),                00024160
     1 XP(300),YP(300),EP(300,2),HP(300),DP(300),VP(300),TP(300),       00024170
     2 XA(50),YA(50),EA(50,2),SIZE(50),                                 00024180
     3 WD(24),WS(24),TA(24),HMIX(24),PEN(24),                           00024190
     4 AX(7,3),BX(7,3),P(7),SCLAB(7),DTDZ(2),  SECTAN(16),              00024200
     5 XSWC,YSWC,GRID,LX,LY,    A(2),B(2),POLNAM(3,2),CALNAM(7,2),      00024210
     6 ITA,IRD,IWR,IDSK,        D80,D47,D8047,DIST,DELTA,               00024220
     7 ESH(2),PEAK,IBUOY,IRISE,IDWN,EFF,XS,    UINV,WVEC,               00024230
     8 NAS,NPS,INDEX,IGRID,IAV,ISCEN,IWDOPT,IWD,ISC,IPS,                00024240
     9 NTOPT,NWDOPT,NWSOPT,NSCEN,NLIST,NARRAY,NTAPE,NCSOPT,NMAX,        00024250
     * NSTDWN,INTER,NPRINT                                              00024260
C                                                                       00024270
      COMMON/PARM1/NPOL,ICT,VD1,W1,VD2,W2,TAUC                          00024280
      DIMENSION CON(2),CALCON(2),SD(2),CALSD(2)                         00024290
C                                                                       00024300
C                                                                       00024310
      WOUT= WD(ISCEN)*180./3.1415927                                    00024320
C                                                                       00024330
C   CONTROL STRATEGY RESULTS OUTPUT BY SUBROUTINE WOROUT                00024340
      IF(NCSOPT.GT.0.AND.NTOPT.EQ.1) CALL WOROUT                        00024350
C                                                                       00024360
C  PRINT AND/OR WRITE-ON-TAPE LISTS OF CONCENTRATION(S) AND             00024370
C     SURFACE DEPOSITION FLUX(ES)                                       00024380
      IF(NLIST.EQ.0 .AND. NTAPE.EQ.0) GO TO 350                         00024390
      IF(NTAPE.EQ.1) WRITE(ITA,900)TT                                   00024400
      NREP=0                                                            00024410
C                                                                       00024420
C  BEGIN LOOP ON COLUMNS                                                00024430
  100 DO 325 I=1,LX                                                     00024440
      IF(NLIST.EQ.0) GO TO 250                                          00024450
      ISKIP=0                                                           00024460
      DO 125 JM=1,LY                                                    00024470
      DO 125 KM=1,2                                                     00024480
      IF(CONC(I,JM,KM).NE.0.) GO TO 130                                 00024490
  125 CONTINUE                                                          00024500
      ISKIP=1                                                           00024510
      IF(NTAPE.EQ.0) GO TO 325                                          00024520
      GO TO 250                                                         00024530
  130 IF(NREP.EQ.1) GO TO 150                                           00024540
      WRITE(IWR,905)TT,ISCEN,SCLAB(ISC),WS(ISCEN),WOUT,                 00024550
     1 HMIX(ISCEN),IAV                                                  00024560
      WRITE(IWR,910)(CALNAM(L,1),L=1,7),(CALNAM(L,2),L=1,7),            00024570
     1 (POLNAM(L,1),L=1,3),(POLNAM(L,2),L=1,3),(POLNAM(L,1),L=1,3),     00024580
     2 (POLNAM(L,2),L=1,3)                                              00024590
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      GO TO 250                                                         00024600
  150 WRITE(IWR,907) TT,ISCEN,SCLAB(ISC),WS(ISCEN),WOUT,                00024610
     1 HMIX(ISCEN),IAV                                                  00024620
      WRITE(IWR,912) (CALNAM(L,1),L=1,7), (CALNAM(L,2),L=1,7),          00024630
     1 (POLNAM(L,1),L=1,3),(POLNAM(L,2),L=1,3),(POLNAM(L,1),L=1,3),     00024640
     2 (POLNAM(L,2),L=1,3)                                              00024650
C                                                                       00024660
  250 XI=I                                                              00024670
      X=XSWC+(XI-0.5)*GRID                                              00024680
C  BEGIN LOOP ON ROWS IN THIS COLUMN                                    00024690
      DO 300 J=1,LY                                                     00024700
      YJ=J                                                              00024710
      Y=YSWC+(YJ-0.5)*GRID                                              00024720
C                                                                       00024730
C  INITIALIZE CONCENTRATION AND SDF VARIABLES                           00024740
      DO 260 K=1,2                                                      00024750
      CON(K)=0.                                                         00024760
      CALCON(K)=0.                                                      00024770
      SD(K)=0.                                                          00024780
      CALSD(K)=0.                                                       00024790
  260 CONTINUE                                                          00024800
C  SET CONCENTRATION AND SDF - APPLY CALIBRATION COEFFICIENTS           00024810
      DO 280 K=1,NPOL                                                   00024820
      IF(NREP.EQ.1) GO TO 270                                           00024830
      CON(K)=CONC(I,J,K)                                                00024840
      CALCON(K)= A(K) + B(K) * CON(K)                                   00024850
  270 SD(K)=SDF(I,J,K)                                                  00024860
      CALSD(K)= A(K) + B(K) * SD(K)                                     00024870
  280 CONTINUE                                                          00024880
C                                                                       00024890
      IF(NLIST.EQ.0 .OR. ISKIP.EQ.1) GO TO 290                          00024900
      IF(NREP.EQ.0) WRITE(IWR,970) I,J,X,Y,CON(1),CON(2),               00024910
     1 CALCON(1),CALCON(2)                                              00024920
      IF(NREP.EQ.1) WRITE(IWR,970) I,J,X,Y,SD(1),SD(2),                 00024930
     1 CALSD(1),CALSD(2)                                                00024940
  290 IF(NTAPE.EQ.0 .OR. NREP.EQ.1) GO TO 300                           00024950
      IF(((I-1)/INTER)*INTER.NE.(I-1).OR.((J-1)/INTER)*INTER.NE.        00024960
     1 (J-1)) GO TO 300                                                 00024970
      WRITE(ITA,975)X,Y,(CON(K),SD(K),CALCON(K),CALSD(K),K=1,2)         00024980
300   CONTINUE                                                          00024990
  325 CONTINUE                                                          00025000
C                                                                       00025010
      IF(NLIST.EQ.0 .OR. NREP.EQ.1) GO TO 350                           00025020
C                                                                       00025030
C   IF NO SURF DEP FLUX WAS CALCULATED, SKIP PRINT                      00025040
      IF(VD1.LE.0.01 .AND. VD2.LE.0.01) GO TO 350                       00025050
      NREP=1                                                            00025060
      GO TO 100                                                         00025070
C                                                                       00025080
C  PRINT ARRAY MAPS OF CONCENTRATIONS                                   00025090
350   IF(NARRAY.GT.0) CALL ARRAY                                        00025100
C                                                                       00025110
C  DETERMINE MAXIMUM PREDICTED CONCENTRATION(S) FOR SCENARIO VIA SCENMX 00025120
      IF(NMAX.GT.0.AND.(NTOPT.EQ.1.OR.ISCEN.EQ.NSCEN)) CALL SCENMX      00025130
C                                                                       00025140
      RETURN                                                            00025150
C                                                                       00025160
900   FORMAT(20A4)                                                      00025170
  905 FORMAT(1H1,'PEM OUTPUT:  PREDICTED CONCENTRATION:  ',             00025180
     120A4/' SCENARIO ',I2,', STABILITY=',A2,', WIND SPEED=',F5.2,' M/S,00025190
     2 WIND DIRECTION=',F6.2,' DEG, MIXING HEIGHT=',F7.1,' M, AVERAGING 00025200
     3TIME=',I3,' HR'//)                                                00025210
  907 FORMAT(1H1,'PEM OUTPUT:  PREDICTED SURFACE DEPOSITION FLUX:  ',   00025220
     120A4/' SCENARIO ',I2,', STABILITY=',A2,', WIND SPEED=',           00025230
     2F5.2,' M/S, WIND DIRECTION=',F6.2,' DEG, MIXING HEIGHT=',F7.1,    00025240
     3' M, AVERAGING TIME=',I3,' HR'//)                                 00025250
  910 FORMAT(33X,'UNCALIBRATED CONCENTRATION',11X,'CALIBRATED CONCENTRAT00025260
     1ION  POL-1: ',7A4/16X,'RECEPTOR',9X,'(MICROGRAMS PER CUBIC METER)'00025270
     2,9X,'CALIBRATED CONCENTRATION  POL-2: ',7A4/15X,'COORDINATES',7X, 00025280
     3'POLLUTANT-1',5X,'POLLUTANT-2',10X,'POLLUTANT-1',5X,'POLLUTANT-2'/00025290
     4' COL ROW',6X,'X(KM)',4X,'Y(KM)',5X,3A4,4X,3A4,9X,3A4,4X,3A4)     00025300
  912 FORMAT(32X,'UNCALIBRATED SURFACE DEPOSITION FLUX',4X,'CALIBRATED V00025310
     1ALUE  POLLUTANT-1: ',7A4/16X,'RECEPTOR',9X,'(MICROGRAMS PER SQ MET00025320
     2ER PER HOUR)',5X,'CALIBRATED VALUE  POLLUTANT-2: ',7A4/           00025330
     315X,'COORDINATES',7X,'POLLUTANT-1',5X,'POLLUTANT-2',12X,          00025340
     4'POLLUTANT-1',5X,'POLLUTANT-2'/' COL ROW',6X,'X(KM)',4X,'Y(KM)',  00025350
     55X,3A4,4X,3A4,11X,3A4,4X,3A4)                                     00025360
  970 FORMAT(2(2X,I2),2X,F9.2,F9.2,6X,F11.4,5X,F11.4,10X,F11.4,5X,F11.4)00025370
  975 FORMAT(10F8.2)                                                    00025380
      END                                                               00025390
C                                                                       00025400
      SUBROUTINE ARRAY                                                  00025410
C                                                                       00025420
C                      SUBROUTINE ARRAY  (VERSION 82360), PART OF PEM.  00025430
C                                                                       00025440
C                                                                       00025450
C  SUBROUTINE ARRAY CREATES ARRAY MAPS OF THE CONCENTRATIONS AND        00025460
C    SURFACE DEPOSITION FLUXES IN THE RECEPTOR GRID AND                 00025470
C    PRINTS THEM AT THE END OF EACH SCENARIO.                           00025480
C    UNCALIBRATED AND CALIBRATED CONCENTRATIONS OF EACH POLLUTANT       00025490
C    APPEAR ON SEPARATE MAPS OF UP TO FOUR SECTIONS (PAGES) EACH.       00025500
C                                                                       00025510
C                                                                       00025520
C *** PEM MODIFICATIONS AND FORMATS BY M.M. STEVENS,                    00025530
C     NOAA-ATDL, P.O. BOX E, OAK RIDGE, TN 37830                        00025540
C     DECEMBER 1982                                                     00025550
C                                                                       00025560
C                                                                       00025570
      COMMON/PEMCOM/CONC(50,50,2),SDF(50,50,2),  TT(20),                00025580
     1 XP(300),YP(300),EP(300,2),HP(300),DP(300),VP(300),TP(300),       00025590
     2 XA(50),YA(50),EA(50,2),SIZE(50),                                 00025600
     3 WD(24),WS(24),TA(24),HMIX(24),PEN(24),                           00025610
     4 AX(7,3),BX(7,3),P(7),SCLAB(7),DTDZ(2),  SECTAN(16),              00025620
     5 XSWC,YSWC,GRID,LX,LY,    A(2),B(2),POLNAM(3,2),CALNAM(7,2),      00025630
     6 ITA,IRD,IWR,IDSK,        D80,D47,D8047,DIST,DELTA,               00025640
     7 ESH(2),PEAK,IBUOY,IRISE,IDWN,EFF,XS,    UINV,WVEC,               00025650
     8 NAS,NPS,INDEX,IGRID,IAV,ISCEN,IWDOPT,IWD,ISC,IPS,                00025660
     9 NTOPT,NWDOPT,NWSOPT,NSCEN,NLIST,NARRAY,NTAPE,NCSOPT,NMAX,        00025670
     * NSTDWN,INTER,NPRINT                                              00025680
C                                                                       00025690
      COMMON/PARM1/NPOL,ICT,VD1,W1,VD2,W2,TAUC                          00025700
      DIMENSION X(50),CC(50),SSDF(50),DV(2)                             00025710
      INTEGER CC,SSDF                                                   00025720
C                                                                       00025730
      DV(1)=VD1                                                         00025740
      DV(2)=VD2                                                         00025750
      WOUT= WD(ISCEN)*180./3.1415927                                    00025760
      NLX=1                                                             00025770
      NLY=1                                                             00025780
      IF(LX.GT.25) NLX=2                                                00025790
      IF(LY.GT.25) NLY=2                                                00025800
      NSECT=NLX*NLY                                                     00025810
C                                                                       00025820
  100 ISECT=0                                                           00025830
      DO 700 JLX=1,NLX                                                  00025840
      MX2= JLX*25                                                       00025850
      IF(MX2.GT.LX) MX2=LX                                              00025860
      MX1=1                                                             00025870
      IF(JLX.EQ.2) MX1=26                                               00025880
      DO 125 I=MX1,MX2                                                  00025890
      XI=I                                                              00025900
  125 X(I)= XSWC + (XI-0.5)*GRID                                        00025910
      DO 600 JLY=1,NLY                                                  00025920
      ISECT=ISECT+1                                                     00025930
      IF(JLY.EQ.1) GO TO 150                                            00025940
      MY1=26                                                            00025950
      MY2=LY                                                            00025960
      GO TO 175                                                         00025970
  150 MY1=1                                                             00025980
      MY2=25                                                            00025990
      IF(LY.LT.25) MY2=LY                                               00026000
  175 DO 500 N=1,NPOL                                                   00026010
      NREP=0                                                            00026020
  180 IF(NARRAY.EQ.3) GO TO 320                                         00026030
      WRITE(IWR,900)ISECT,NSECT,ISCEN,TT                                00026040
      WRITE(IWR,902)SCLAB(ISC),WS(ISCEN),WOUT,HMIX(ISCEN),IAV,          00026050
     1          N,(POLNAM(L,N),L=1,3)                                   00026060
      IF(NREP.EQ.0) GO TO 185                                           00026070
C     LOOP THROUGH SDF ARRAY TO FIND ANY VALUE GE 1000. IN THAT CASE,   00026080
C      SET FLAG TO SCALE SDF VALUES AS THEY ARE SET IN SSDF ARRAY       00026090
      IFLAG=0                                                           00026100
      DO 182 NX=1,LX                                                    00026110
      DO 182 NY=1,LY                                                    00026120
      IF(SDF(NX,NY,N).GT.999.49) GO TO 184                              00026130
  182 CONTINUE
      WRITE(IWR,905)
      GO TO 190
  184 IFLAG=1
      WRITE(IWR,910)
      GO TO 190
  185 WRITE(IWR,904)
  190 WRITE(IWR,915) (X(I),I=MX1,MX2,2)
      DO 300 J=MY1,MY2
      IY= MY2 + MY1 - J
      Y=IY
      Y= YSWC + (Y-0.5)*GRID
C
      IF(NREP.EQ.1) GO TO 240
      DO 230 I=MX1,MX2
230   CC(I)= CONC(I,IY,N) + 0.5
      WRITE(IWR,920)Y,(CC(I),I=MX1,MX2)
      GO TO 300
  240 DO 250 I=MX1,MX2
      IF(IFLAG.EQ.0) GO TO 245
      SSDF(I)=SDF(I,IY,N)*1.0E-03 + 0.5
      GO TO 250
  245 SSDF(I)= SDF(I,IY,N) + 0.5
  250 CONTINUE
      WRITE(IWR,920) Y,(SSDF(I),I=MX1,MX2)
300   WRITE(IWR,925)Y
      WRITE(IWR,915)(X(I),I=MX1,MX2,2)
320   IF(NARRAY.EQ.2) GO TO 450
      WRITE(IWR,900)ISECT,NSECT,ISCEN,TT
      WRITE(IWR,902)SCLAB(ISC),WS(ISCEN),WOUT,HMIX(ISCEN),IAV,
     1              N,(POLNAM(L,N),L=1,3)
      IF(NREP.EQ.0) WRITE(IWR,906)(CALNAM(L,N),L=1,7),A(N),B(N)
      IF(NREP.EQ.1) WRITE(IWR,907) (CALNAM(L,N),L=1,7),A(N),B(N)
      WRITE(IWR,915)(X(I),I=MX1,MX2,2)
      DO 400 J=MY1,MY2
      IY= MY2 + MY1 - J
      Y=IY
      Y= YSWC + (Y-0.5)*GRID
C
      IF(NREP.EQ.1) GO TO 340
      DO 330 I=MX1,MX2
330   CC(I)= A(N) + B(N)*CONC(I,IY,N) + 0.5
      WRITE(IWR,920)Y,(CC(I),I=MX1,MX2)
      GO TO 400
  340 DO 350 I=MX1,MX2
  350 SSDF(I)= A(N) + B(N) * SDF(I,IY,N) + 0.5
      WRITE(IWR,920) Y,(SSDF(I),I=MX1,MX2)
400   WRITE(IWR,925)Y
      WRITE(IWR,915)(X(I),I=MX1,MX2,2)
  450 IF(NREP.EQ.1) GO TO 500
C   IF NO SURF DEP FLUX WAS CALCULATED, SKIP PRINT
      IF(DV(N).LE.0.01) GO TO 500
      NREP=1
      GO TO 180
500   CONTINUE
600   CONTINUE
700   CONTINUE
C
      RETURN
C
900    FORMAT(1H1,'PEM OUTPUT:  ','SECTION ',I1,' OF ',I1,', SCENARIO ',
     1 I2,2X,20A4)
902    FORMAT(' STABILITY=',A2,', WIND SPD=',F5.2,' M/S, WIND DIR=',F6.2,
     1 ' DEG, MIXING HT=',F7.1,' M, AVERAGING TIME=',I3,' HR.',6X,
     2 'POLLUTANT-',I1,': ',3A4)
904    FORMAT(' UNCALIBRATED CONCENTRATION - MICROGRAMS PER CUBIC METER')
  905 FORMAT(' UNCALIBRATED SURFACE DEPOSITION FLUX - MICROGRAMS PER SQU
     1ARE METER PER HOUR')
906    FORMAT(' CALIBRATED CONCENTRATION - ',7A4,18X,'CALIBRATION COEFFIC
     1IENTS:  A =',F11.4,',  B =',F11.4)
  907 FORMAT(' CALIBRATED SURFACE DEPOSITION FLUX - ',7A4,10X,
     1'CALIBRATION COEFFICIENTS:  A=',F10.4,5X,'B=',F10.4)
  910 FORMAT(' UNCALIBRATED SURFACE DEPOSITION FLUX - KILOGRAMS PER SQUA
     1RE KILOMETER PER HOUR')
915   FORMAT(1H0,14X,13F8.2)
920   FORMAT(1H0,4X,F8.2,4X,25I4)
925   FORMAT(1H+,122X,F8.2)
```

```
      END                                                               00026910
C                                                                       00026920
C                                                                       00026930
      SUBROUTINE WORST(I,J,CHI)                                         00026940
C                        SUBROUTINE WORST  (VERSION 82360), PART OF PEM.00026950
C                                                                       00026960
C                                                                       00026970
C  SUBROUTINE WORST DETERMINES THE FIVE POINT SOURCES CONTRIBUTING THE  00026980
C    MOST TO THE TOTAL CONCENTRATION AT EACH RECEPTOR. SOURCE           00026990
C    IDENTIFICATIONS AND CONTRIBUTIONS ARE STORED IN NWORST AND CWORST  00027000
C    RESPECTIVELY, FOR OUTPUT BY SUBROUTINE WOROUT.                     00027010
C                                                                       00027020
C                                                                       00027030
C *** PEM MODIFICATIONS BY M.M. STEVENS,                                00027040
C      NOAA-ATDL, P.O. BOX-E, OAK RIDGE, TENN 37830                     00027050
C      DECEMBER 1982                                                    00027060
C                                                                       00027070
C                                                                       00027080
      COMMON/PEMCOM/CONC(50,50,2),SDF(50,50,2),  TT(20),                00027090
     1 XP(300),YP(300),EP(300,2),HP(300),DP(300),VP(300),TP(300),       00027100
     2 XA(50),YA(50),EA(50,2),SIZE(50),                                 00027110
     3 WD(24),WS(24),TA(24),HMIX(24),PEN(24),                           00027120
     4 AX(7,3),BX(7,3),P(7),SCLAB(7),DTDZ(2),  SECTAN(16),              00027130
     5 XSWC,YSWC,GRID,LX,LY,    A(2),B(2),POLNAM(3,2),CALNAM(7,2),      00027140
     6 ITA,IRD,IWR,IDSK,        D80,D47,D8047,DIST,DELTA,               00027150
     7 ESH(2),PEAK,IBUOY,IRISE,IDWN,EFF,XS,    UINV,WVEC,               00027160
     8 NAS,NPS,INDEX,IGRID,IAV,ISCEN,IWDOPT,IWD,ISC,IPS,                00027170
     9 NTOPT,NWDOPT,NWSOPT,NSCEN,NLIST,NARRAY,NTAPE,NCSOPT,NMAX,        00027180
     * NSTDWN,INTER,NPRINT                                              00027190
C                                                                       00027200
      COMMON/CSWOR/NWORST(25,25,5),CWORST(25,25,5)                      00027210
C                                                                       00027220
C                                                                       00027230
      IF(CHI.LE.CWORST(I,J,5)) RETURN                                   00027240
      IF(CHI.GT.CWORST(I,J,4)) GO TO 205                                00027250
      CWORST(I,J,5)= CHI                                                00027260
      NWORST(I,J,5)= IPS                                                00027270
      RETURN                                                            00027280
  205 IF(CHI.GT.CWORST(I,J,3)) GO TO 210                                00027290
      NW=1                                                              00027300
      GO TO 225                                                         00027310
  210 IF(CHI.GT.CWORST(I,J,2)) GO TO 215                                00027320
      NW=2                                                              00027330
      GO TO 225                                                         00027340
  215 IF(CHI.GT.CWORST(I,J,1)) GO TO 220                                00027350
      NW=3                                                              00027360
      GO TO 225                                                         00027370
  220 NW=4                                                              00027380
  225 DO 250 IW=1,NW                                                    00027390
      CWORST(I,J,6-IW)= CWORST(I,J,5-IW)                                00027400
  250 NWORST(I,J,6-IW)= NWORST(I,J,5-IW)                                00027410
      CWORST(I,J,5-NW)= CHI                                             00027420
      NWORST(I,J,5-NW)= IPS                                             00027430
      RETURN                                                            00027440
      END                                                               00027450
C                                                                       00027460
C                                                                       00027470
      SUBROUTINE WOROUT                                                 00027480
C                        SUBROUTINE WOROUT (VERSION 82350), PART OF PEM.00027490
C                                                                       00027500
C                                                                       00027510
C  SUBROUTINE WOROUT PRINTS A CULPABILITY LIST OF THE IDENTIFICATIONS   00027520
C    AND CONTRIBUTIONS OF THE FIVE POINT SOURCES CONTRIBUTING THE MOST  00027530
C    TO THE TOTAL CONCENTRATION AND SURFACE DEPOSITION FLUX AT EACH     00027540
C    RECEPTOR, USING DATA COMPILED BY SUBROUTINE WORST                  00027550
C                                                                       00027560
C                                                                       00027570
C *** PEM MODIFICATIONS AND FORMATS BY M.M. STEVENS,                    00027580
C      NOAA-ATDL, P.O. BOX E, OAK RIDGE, TN 37830                       00027590
C      DECEMBER 1982                                                    00027600
C                                                                       00027610
C                                                                       00027620
      COMMON/PEMCOM/CONC(50,50,2),SDF(50,50,2),  TT(20),                00027630
     1 XP(300),YP(300),EP(300,2),HP(300),DP(300),VP(300),TP(300),       00027640
     2 XA(50),YA(50),EA(50,2),SIZE(50),                                 00027650
     3 WD(24),WS(24),TA(24),HMIX(24),PEN(24),                           00027660
     4 AX(7,3),BX(7,3),P(7),SCLAB(7),DTDZ(2),  SECTAN(16),              00027670
     5 XSWC,YSWC,GRID,LX,LY,    A(2),B(2),POLNAM(3,2),CALNAM(7,2),
     6 ITA,IRD,IWR,IDSK,           D80,D47,D8047,DIST,DELTA,
     7 ESH(2),PEAK,IBUOY,IRISE,IDWN,EFF,XS,    UINV,WVEC,
     8 NAS,NPS,INDEX,IGRID,IAV,ISCEN,IWDOPT,IWD,ISC,IPS,
     9 NTOPT,NWDOPT,NWSOPT,NSCEN,NLIST,NARRAY,NTAPE,NCSOPT,NMAX,
     * NSTDWN,INTER,NPRINT
C
      COMMON/CSWOR/NWORST(25,25,5),CWORST(25,25,5)
C
C
      WOUT= WD(ISCEN)*180./3.1415927
      N=1
      IF(NTOPT.EQ.1) GO TO 250
      N=2
250   DO 400 I=1,LX
C    IF ALL CONCENTRATION VALUES ARE ZERO IN THIS COL, SKIP IT
      DO 275 JM=1,LY
      IF(CONC(I,JM,N).NE.0.) GO TO 280
  275 CONTINUE
      GO TO 400
C
  280 WRITE(IWR,905) TT,(POLNAM(L,1),L=1,3)
      WRITE(IWR,910) ISCEN,WOUT,WS(ISCEN),SCLAB(ISC),HMIX(ISCEN),IAV
      WRITE(IWR,915)
      XI=I
      X= XSWC + (XI-0.5)*GRID
      DO 400 J=1,LY
      IF(CONC(I,J,N).LT.1.0E-5) GO TO 303
      DO 300 L=1,5
300   CWORST(I,J,L)= CWORST(I,J,L)*100./CONC(I,J,N)
303   YJ=J
      Y= YSWC + (YJ-0.5)*GRID
      WRITE(IWR,925)I,J,X,Y,NWORST(I,J,1),CWORST(I,J,1),NWORST(I,J,2),
     1 CWORST(I,J,2),NWORST(I,J,3),CWORST(I,J,3),NWORST(I,J,4),
     2 CWORST(I,J,4),NWORST(I,J,5),CWORST(I,J,5),CONC(I,J,N),SDF(I,J,N)
400   CONTINUE
C
      RETURN
C
  905 FORMAT(1H1,45X,'POLLUTION EPISODIC MODEL'///4X,'OUTPUT:  ',20A4//
     14X,'LIST OF THE FIVE POINT SOURCES WHICH PRODUCE THE HIGHEST VALUE
     2S OF CONCENTRATION AND SURFACE DEPOSITION FLUX AT EACH RECEPTOR'//
     34X,'POLLUTANT: ',3A4,'  -  CONCENTRATION IN MICROGRAMS PER CUBIC M
     4ETER'/32X,'SURFACE DEPOSITION FLUX IN MICROGRAMS PER SQUARE METER 
     5PER HOUR'/)
  910 FORMAT(4X,'SCENARIO',6X,'WIND DIRECTION',6X,'WIND SPEED',6X,'STABI
     1LITY CLASS',6X,'MIXING HEIGHT',6X,'AVERAGING TIME'/
     25X,'NUMBER',11X,'(DEG)',13X,'(M/S)',34X,'(M)',17X,'(HR)'/
     37X,I2,13X,F5.1,13X,F5.2,15X,A2,15X,F7.2,15X,I3/)
  915 FORMAT(45X,'POINT SOURCE SEQUENCE NUMBER AND PERCENT'/
     115X,'COORDINATES',15X,'OF TOTAL CONCENTRATION AND SURFACE DEPOSITI
     2ON FLUX',14X,'TOTAL',8X,'TOTAL SURFACE'/
     3' COL ROW',4X,'X (KM)',4X,'Y (KM)',9X,'HIGHEST',6X,'SECOND',8X,
     4'THIRD',7X,'FOURTH',8X,'FIFTH',6X,'CONCENTRATION',3X,'DEPOSITION F
     5LUX'/)
  925 FORMAT(2(2X,I2),3X,F8.2,2X,F8.2,3X,5(3X,I3,F7.2),6X,F8.2,9X,F8.2)
C
      END
C
C
      SUBROUTINE SCENMX
C                    SUBROUTINE SCENMX (VERSION 82360), PART OF PEM.
C
C
C  SUBROUTINE SCENMX LOCATES AND STORES THE COORDINATES, CONCENTRATION,
C  AND SURFACE DEPOSITION FLUX AT THE RECEPTOR GRID POINTS RECORDING
C  THE HIGHEST CONCENTRATION AND SURFACE DEPOSITION FLUX OF EACH
C  POLLUTANT IN EACH SCENARIO.  STORED VALUES ARE PRINTED BY SUBROUTINE
C  MAXOUT AT THE END OF THE RUN.
C
C
C *** PEM MODIFICATIONS BY M.M. STEVENS,
C     NOAA-ATDL, P.O.BOX - E, OAK RIDGE, TN 37830
C     DECEMBER 1982
C
C
      COMMON/PEMCOM/CONC(50,50,2),SDF(50,50,2),  TT(20),
     1 XP(300),YP(300),EP(300,2),HP(300),DP(300),VP(300),TP(300),       00028450
     2 XA(50),YA(50),EA(50,2),SIZE(50),                                  00028460
     3 WD(24),WS(24),TA(24),HMIX(24),PEN(24),                            00028470
     4 AX(7,3),BX(7,3),P(7),SCLAB(7),DTDZ(2),  SECTAN(16),               00028480
     5 XSWC,YSWC,GRID,LX,LY,    A(2),B(2),POLNAM(3,2),CALNAM(7,2),       00028490
     6 ITA,IRD,IWR,IDSK,        D80,D47,D8047,DIST,DELTA,                00028500
     7 ESH(2),PEAK,IBUOY,IRISE,IDWN,EFF,XS,    UINV,WVEC,                00028510
     8 NAS,NPS,INDEX,IGRID,IAV,ISCEN,IWDOPT,IWD,ISC,IPS,                 00028520
     9 NTOPT,NWDOPT,NWSOPT,NSCEN,NLIST,NARRAY,NTAPE,NCSOPT,NMAX,         00028530
     * NSTDWN,INTER,NPRINT                                               00028540
C                                                                        00028550
      COMMON/MAX/XMX(24,4,2),YMX(24,4,2),ZMX(24,4,2),SMX(24,4,2)         00028560
      COMMON/PARM1/NPOL,ICT,VD1,W1,VD2,W2,TAUC                           00028570
C                                                                        00028580
C                                                                        00028590
      IF(NTOPT.EQ.1) GO TO 120                                           00028600
      I= 1                                                               00028610
      GO TO 130                                                          00028620
120   I= ISCEN                                                           00028630
130   IF(NWDOPT.LE.1) GO TO 140                                          00028640
      J= IWDOPT                                                          00028650
      GO TO 150                                                          00028660
140   J= 1                                                               00028670
150   DO 400 K=1,NPOL                                                    00028680
      Z= 0.                                                              00028690
      DO 350 NX=1,LX                                                     00028700
      DO 350 NY=1,LY                                                     00028710
      IF(CONC(NX,NY,K).LT.Z) GO TO 350                                   00028720
      Z= CONC(NX,NY,K)                                                   00028730
      ZS=SDF(NX,NY,K)                                                    00028740
      ZX=NX                                                              00028750
      ZY=NY                                                              00028760
 350  CONTINUE                                                           00028770
      ZMX(I,J,K)= Z                                                      00028780
      SMX(I,J,K)=ZS                                                      00028790
      XMX(I,J,K)= XSWC + (ZX - 0.5)*GRID                                 00028800
      YMX(I,J,K)= YSWC + (ZY - 0.5)*GRID                                 00028810
 400  CONTINUE                                                           00028820
      RETURN                                                             00028830
      END                                                                00028840
C                                                                        00028850
C                                                                        00028860
      SUBROUTINE MAXOUT                                                  00028870
C                     SUBROUTINE MAXOUT (VERSION 82350), PART OF PEM.    00028880
C                                                                        00028890
C                                                                        00028900
C  SUBROUTINE MAXOUT PRINTS THE COORDINATES, CONCENTRATION, AND          00028910
C  SURFACE DEPOSITION FLUX AT THE RECEPTOR GRID POINTS RECORDING         00028920
C  THE HIGHEST CONCENTRATION OF EACH POLLUTANT IN EACH SCENARIO.         00028930
C  THESE VALUES WERE SELECTED AND STORED BY SUBROUTINE SCENMX.           00028940
C                                                                        00028950
C                                                                        00028960
C                                                                        00028970
C *** PEM MODIFICATIONS AND FORMATS BY M.M. STEVENS,                     00028980
C     NOAA-ATDL, P.O.BOX E, OAK RIDGE, TN 37830                          00028990
C     DECEMBER 1982                                                      00029000
C                                                                        00029010
C                                                                        00029020
      COMMON/PEMCOM/CONC(50,50,2),SDF(50,50,2),  TT(20),                 00029030
     1 XP(300),YP(300),EP(300,2),HP(300),DP(300),VP(300),TP(300),       00029040
     2 XA(50),YA(50),EA(50,2),SIZE(50),                                  00029050
     3 WD(24),WS(24),TA(24),HMIX(24),PEN(24),                            00029060
     4 AX(7,3),BX(7,3),P(7),SCLAB(7),DTDZ(2),  SECTAN(16),               00029070
     5 XSWC,YSWC,GRID,LX,LY,    A(2),B(2),POLNAM(3,2),CALNAM(7,2),       00029080
     6 ITA,IRD,IWR,IDSK,        D80,D47,D8047,DIST,DELTA,                00029090
     7 ESH(2),PEAK,IBUOY,IRISE,IDWN,EFF,XS,    UINV,WVEC,                00029100
     8 NAS,NPS,INDEX,IGRID,IAV,ISCEN,IWDOPT,IWD,ISC,IPS,                 00029110
     9 NTOPT,NWDOPT,NWSOPT,NSCEN,NLIST,NARRAY,NTAPE,NCSOPT,NMAX,         00029120
     * NSTDWN,INTER,NPRINT                                               00029130
C                                                                        00029140
      COMMON/MAX/XMX(24,4,2),YMX(24,4,2),ZMX(24,4,2),SMX(24,4,2)         00029150
      COMMON/PARM1/NPOL,ICT,VD1,W1,VD2,W2,TAUC                           00029160
      DIMENSION ZC(2),ZS(2)                                              00029170
C                                                                        00029180
C   CHECK WHETHER SURF DEP FLUX WAS CALCULATED AND SET FLAG              00029190
      NREP=1                                                             00029200
      IF(VD1.LE.0.01 .AND. VD2.LE.0.01) NREP=0                           00029210
```

```
C
      IF(NWDOPT.GT.1) GO TO 300                                         00029220
C                                                                       00029230
      J=1                                                               00029240
      N=1                                                               00029250
      IF(NTOPT.EQ.1) N=NSCEN                                            00029260
C   PRINT HIGHEST CONCENTRATIONS                                        00029270
      WRITE(IWR,900) TT                                                 00029280
      WRITE(IWR,902) (CALNAM(L,1),L=1,7)                                00029290
      IF(NPOL.EQ.2) WRITE(IWR,903) (CALNAM(L,2),L=1,7)                  00029300
      WRITE(IWR,910) (POLNAM(L,1),L=1,3)                                00029310
      IF(NPOL.EQ.2) WRITE(IWR,911) (POLNAM(L,2),L=1,3)                  00029320
      WRITE(IWR,912)                                                    00029330
      WRITE(IWR,915)                                                    00029340
      DO 200 I=1,N                                                      00029350
      DO 120 K=1,NPOL                                                   00029360
  120 ZC(K)= A(K) + B(K)*ZMX(I,1,K)                                     00029370
      WRITE(IWR,920)                                                    00029380
      WRITE(IWR,925) I,J,(XMX(I,1,K),YMX(I,1,K),ZMX(I,1,K),ZC(K),       00029390
     1 K=1,NPOL)                                                        00029400
  200 CONTINUE                                                          00029410
C                                                                       00029420
C   PRINT SURFACE DEPOSITION FLUX VALUES                                00029430
C   IF NO SURF DEP FLUX WAS CALCULATED, SKIP PRINT                      00029440
      IF(NREP.EQ.0) RETURN                                              00029450
      WRITE(IWR,900) TT                                                 00029460
      WRITE(IWR,932) (CALNAM(L,1),L=1,7)                                00029470
      IF(NPOL.EQ.2) WRITE(IWR,933) (CALNAM(L,2),L=1,7)                  00029480
      WRITE(IWR,910) (POLNAM(L,1),L=1,3)                                00029490
      IF(NPOL.EQ.2) WRITE(IWR,911) (POLNAM(L,2),L=1,3)                  00029500
      WRITE(IWR,942)                                                    00029510
      WRITE(IWR,915)                                                    00029520
      DO 250 I=1,N                                                      00029530
      DO 220 K=1,NPOL                                                   00029540
  220 ZS(K)= A(K) + B(K)*SMX(I,1,K)                                     00029550
      WRITE(IWR,920)                                                    00029560
      WRITE(IWR,925) I,J,(XMX(I,1,K),YMX(I,1,K),SMX(I,1,K),ZS(K),       00029570
     1 K=1,NPOL)                                                        00029580
  250 CONTINUE                                                          00029590
C                                                                       00029600
      RETURN                                                            00029610
C                                                                       00029620
C   PRINT FOR CASE OF NWDOPT>1  -  SUB-SCENARIOS                        00029630
  300 N=NSCEN                                                           00029640
C   PRINT HIGHEST CONCENTRATIONS                                        00029650
      DO 500 I=1,N                                                      00029660
      IF(((I-1)/8)*8.NE.I-1) GO TO 310                                  00029670
      WRITE(IWR,900) TT                                                 00029680
      WRITE(IWR,902) (CALNAM(L,1),L=1,7)                                00029690
      IF(NPOL.EQ.2) WRITE(IWR,903) (CALNAM(L,2),L=1,7)                  00029700
      WRITE(IWR,910) (POLNAM(L,1),L=1,3)                                00029710
      IF(NPOL.EQ.2) WRITE(IWR,911) (POLNAM(L,2),L=1,3)                  00029720
      WRITE(IWR,912)                                                    00029730
      WRITE(IWR,915)                                                    00029740
  310 WRITE(IWR,920)                                                    00029750
      DO 400 J=1,4                                                      00029760
      DO 320 K=1,NPOL                                                   00029770
  320 ZC(K)= A(K) + B(K)*ZMX(I,J,K)                                     00029780
      WRITE(IWR,925) I,J,(XMX(I,J,K),YMX(I,J,K),ZMX(I,J,K),ZC(K),       00029790
     1 K=1,NPOL)                                                        00029800
  400 CONTINUE                                                          00029810
  500 CONTINUE                                                          00029820
C                                                                       00029830
C   PRINT SURFACE DEPOSITION FLUX VALUES                                00029840
C   IF NO SURF DEP FLUX WAS CALCULATED, SKIP PRINT                      00029850
      IF(NREP.EQ.0) RETURN                                              00029860
      DO 600 I=1,N                                                      00029870
      IF(((I-1)/8)*8.NE.I-1) GO TO 510                                  00029880
      WRITE(IWR,900) TT                                                 00029890
      WRITE(IWR,932) (CALNAM(L,1),L=1,7)                                00029900
      IF(NPOL.EQ.2) WRITE(IWR,933) (CALNAM(L,2),L=1,7)                  00029910
      WRITE(IWR,910) (POLNAM(L,1),L=1,3)                                00029920
      IF(NPOL.EQ.2) WRITE(IWR,911) (POLNAM(L,2),L=1,3)                  00029930
      WRITE(IWR,942)                                                    00029940
      WRITE(IWR,915)                                                    00029950
  510 WRITE(IWR,920)                                                    00029960
      DO 550 J=1,4                                                      00029970
                                                                        00029980
      DO 520 K=1,NPOL
  520 ZS(K)= A(K) + B(K)*SMX(I,J,K)
      WRITE(IWR,925) I,J,(XMX(I,J,K),YMX(I,J,K),SMX(I,J,K),ZS(K),
     1 K=1,NPOL)
  550 CONTINUE
  600 CONTINUE
C
  700 RETURN
C
  900 FORMAT(1H1,45X,'POLLUTION EPISODIC MODEL'///4X,'OUTPUT:  ',20A4//)
  902 FORMAT(4X,'HIGHEST PREDICTED CONCENTRATION OF EACH POLLUTANT FOR E
     1ACH SCENARIO'//4X,'UNCALIBRATED CONCENTRATION IN MICROGRAMS PER CU
     2BIC METER  -  CALIBRATION, POLLUTANT-1: ',7A4)
  903 FORMAT(65X,'CALIBRATION, POLLUTANT-2: ',7A4)
  910 FORMAT(//40X,'POLLUTANT-1: ',3A4)
  911 FORMAT(1H+,93X,'POLLUTANT-2: ',3A4)
  912 FORMAT(/' SCENARIO  WIND DIRECTION',7X,'COORDINATES',14X,
     1'CONCENTRATION',16X,'COORDINATES',14X,'CONCENTRATION')
  915 FORMAT(2X,'NUMBER',4X,'SUB-SCENARIO',6X,'X(KM)',5X,'Y(KM)',6X,
     1'UNCALIBRATED',4X,'CALIBRATED',7X,'X(KM)',5X,'Y(KM)',6X,
     2'UNCALIBRATED',4X,'CALIBRATED'/)
  920 FORMAT(1X)
  925 FORMAT(4X,I2,11X,I2,8X,F9.2,1X,F9.2,5X,F11.4,4X,F11.4,4X,F9.2,1X,
     1F9.2,5X,F11.4,4X,F11.4)
  932 FORMAT(4X,'HIGHEST PREDICTED SURFACE DEPOSITION FLUX OF EACH POLLU
     1TANT FOR EACH SCENARIO'//4X,'UNCALIBRATED VALUES IN MICROGRAMS PER
     2 SQUARE METER PER HOUR  -  CALIBRATION, POLLUTANT-1: ',7A4)
  933 FORMAT(68X,'CALIBRATION, POLLUTANT-2: ',7A4)
  942 FORMAT(/' SCENARIO  WIND DIRECTION',7X,'COORDINATES',9X,
     1'SURFACE DEPOSITION FLUX',11X,'COORDINATES',9X,'SURFACE DEPOSITION
     2 FLUX')
      END
C
C
      SUBROUTINE RISE
C
C                        SUBROUTINE RISE   (VERSION 82360), PART OF PEM.
C
C
C SUBROUTINE RISE CALCULATES PLUME RISE VIA ONE OF SIX EQUATIONS
C    (BRIGGS,1969). IF IRISE=1, DISTANCE DEPENDENT EFFECTIVE SOURCE
C    HEIGHT (ESH(1)) IS RETURNED. IF IRISE=2, MAXIMUM EFFECTIVE SOURCE
C    HEIGHT (ESH(2)) IS RETURNED. RISE IS CALLED ONCE PER SOURCE PER
C    SCENARIO WITH IRISE=2. IT IS CALLED WITH IRISE=1 WHENEVER THE
C    DOWNWIND DISTANCE (DIST) IS LESS THAN THE DISTANCE TO MAXIMUM
C    PLUME RISE (PEAK).
C
C
      COMMON/PEMCOM/CONC(50,50,2),SDF(50,50,2),  TT(20),
     1 XP(300),YP(300),EP(300,2),HP(300),DP(300),VP(300),TP(300),
     2 XA(50),YA(50),EA(50,2),SIZE(50),
     3 WD(24),WS(24),TA(24),HMIX(24),PEN(24),
     4 AX(7,3),BX(7,3),P(7),SCLAB(7),DTDZ(2),  SECTAN(16),
     5 XSWC,YSWC,GRID,LX,LY,     A(2),B(2),POLNAM(3,2),CALNAM(7,2),
     6 ITA,IRD,IWR,IDSK,        D80,D47,D8047,DIST,DELTA,
     7 ESH(2),PEAK,IBUOY,IRISE,IDWN,EFF,XS,    UINV,WVEC,
     8 NAS,NPS,INDEX,IGRID,IAV,ISCEN,IWDOPT,IWD,ISC,IPS,
     9 NTOPT,NWDOPT,NWSOPT,NSCEN,NLIST,NARRAY,NTAPE,NCSOPT,NMAX,
     * NSTDWN,INTER,NPRINT
C
      IDWN=1
      IF(IRISE.EQ.1) GO TO 300
      DWNWSH= 1.0
      IF(IBUOY.EQ.0) GO TO 205
      IF(EFF.GE.55.) GO TO 150
C
C  XS,CTB, AND CTMU ARE INDEPENDENT OF DISTANCE, AND ARE THEREFORE
C     CALCULATED ONCE PER SOURCE PER SCENARIO (WHEN IRISE=2).
      XS= 49.*EFF**0.625
      GO TO 160
  150 XS=119.*EFF**0.4
  160 CTB= 1.6*UINV*EFF**0.333333
      IF(ISC.GE.6) GO TO 170
C
C PEAK PLUME RISE: BUOYANCY-DOMINATED PLUME, UNSTABLE AIR (A-D).
      DELTAH= CTB*XS**0.666667
      GO TO 250
C
```

```
C  PEAK PLUME RISE: BUOYANCY-DOMINATED PLUME, STABLE AIR (E,F).
170   DELTAH= 2.6*(EFF*UINV*TA(ISCEN)/(9.8*DTDZ(ISC-5)))**0.333333
      GO TO 250
205   IF(ISC.GE.6) GO TO 230
      CTMU= 1.89*(VP(IPS)*VP(IPS)*DP(IPS)*UINV/(VP(IPS)+3./UINV))**0.666
     1667
C
C  PEAK PLUME RISE: MOMENTUM-DOMINATED PLUME, UNSTABLE AIR (A-D).
      DELTAH= 3.0*VP(IPS)*DP(IPS)*UINV
      GO TO 250
C
C  PEAK PLUME RISE: MOMENTUM-DOMINATED PLUME, STABLE AIR (E,F).
230   DELTAH= 1.5*(0.5*VP(IPS)*DP(IPS))**0.666667*UINV**0.333333
     1 *(TA(ISCEN)/(DTDZ(ISC-5)*9.8))**0.166667
250   IF(NSTDWN.EQ.1) GO TO 270
      IF(VP(IPS)*UINV.GT.1.5) GO TO 270
      CDELH= 2.0*(1.5 - VP(IPS)*UINV)*DP(IPS)
      IDWN=3
      IF(CDELH.GE.DELTAH) GO TO 260
      DWNWSH= (DELTAH-CDELH)/DELTAH
      GO TO 270
260   DWNWSH= 0.
270   ESH(2)= HP(IPS) + DELTAH*DWNWSH
      RETURN
C
300   IF(IBUOY.EQ.0) GO TO 500
C
C  DISTANCE-DEPENDENT PLUME RISE: BUOYANCY-DOMINATED PLUME,
C     ANY STABILITY (A-F).
      ESH(1)= DWNWSH*CTB*(DIST*1000.)**0.666667 + HP(IPS)
      IF(ESH(1).GT.ESH(2)) ESH(1)=ESH(2)
      RETURN
C
C  DISTANCE-DEPENDENT PLUME RISE: MOMENTUM-DOMINATED PLUME,
C     UNSTABLE AIR (A-D).
500   ESH(1)= DWNWSH*CTMU*(DIST*1000.)**0.333333 + HP(IPS)
      IF(ESH(1).GT.ESH(2)) ESH(1)=ESH(2)
      RETURN
C
C  THERE IS NO DISTANCE-DEPENDENT PLUME RISE GIVEN FOR A
C     MOMENTUM-DOMINATED PLUME IN STABLE AIR. DISTANCE TO MAXIMUM PLUME
C     RISE FOR THIS SITUATION IS SET EQUAL TO ZERO IN THE MAIN PROGRAM,
C     SO THE MAXIMUM HEIGHT, ESH(2), IS USED AT ALL DISTANCES.
      END
C
C
C
      SUBROUTINE AUTGRD
                      SUBROUTINE AUTGRD (VERSION 82360), PART OF PEM.
C
C
C
C  SUBROUTINE AUTGRID CALCULATES THE FIVE PARAMETERS DEFINING THE
C     RECEPTOR GRID (XSWC,YSWC,LX,LY,GRID) WHEN THE AUTOMATIC GRID
C     OPTION IS USED. THIS IS DONE BY SETTING GRID=0.0 IN THE INPUT
C     DATA. GRID PARAMETERS WILL BE CHOSEN FOR EACH SCENARIO SO AS
C     TO INSURE GOOD COVERAGE BY RECEPTORS NEAR THE POINT OF
C     MAXIMUM CONCENTRATION.  THIS POINT IS DETERMINED USING GAUSSIAN
C     PLUME ALGORITHMS WITHOUT POLLUTANT REMOVAL MECHANISMS.  THIS
C     POINT IS THEREFORE ONLY APPROXIMATE FOR PROBLEMS WHICH INCLUDE
C     DEPOSITION, SEDIMENTATION, AND CHEMICAL DECAY/TRANSFORMATION.
C     THE OPTIMUM RECEPTOR GRID IN THIS CASE SHOULD BE DETERMINED BY
C     TRIAL AND ERROR, USING THE RECEPTOR GRID DEFINED BY AUTGRD AS
C     THE FIRST APPROXIMATION.
C
C
      COMMON/PEMCOM/CONC(50,50,2),SDF(50,50,2),  TT(20),
     1 XP(300),YP(300),EP(300,2),HP(300),DP(300),VP(300),TP(300),
     2 XA(50),YA(50),EA(50,2),SIZE(50),
     3 WD(24),WS(24),TA(24),HMIX(24),PEN(24),
     4 AX(7,3),BX(7,3),P(7),SCLAB(7),DTDZ(2),  SECTAN(16),
     5 XSWC,YSWC,GRID,LX,LY,    A(2),B(2),POLNAM(3,2),CALNAM(7,2),
     6 ITA,IRD,IWR,IDSK,        D80,D47,D8047,DIST,DELTA,
     7 ESH(2),PEAK,IBUOY,IRISE,IDWN,EFF,XS,    UINV,WVEC,
     8 NAS,NPS,INDEX,IGRID,IAV,ISCEN,IWDOPT,IWD,ISC,IPS,
     9 NTOPT,NWDOPT,NWSOPT,NSCEN,NLIST,NARRAY,NTAPE,NCSOPT,NMAX,
     * NSTDWN,INTER,NPRINT
C
```

```
C
      DIMENSION XCRNR(4),YCRNR(4),HL(2),DL(2),XTM(2)
      DIMENSION AG(7,2),BG(7,2),DG(7)
      DATA AG/.0383,.1393,.112,.0856,.0818,.1094,.05645,
     1        .0002539,.04396,.1014,.2591,.2527,.2452,.1930/
      DATA BG/1.281,.9467,.9100,.865,.8155,.7657,.805,
     1        2.089,1.114,.926,.6869,.6341,.6358,.6072/
      DATA DG/.873,.897,.908,.916,.916,.912,.911/
C
C
      E= 1.570796 -WVEC
      SINEE= SIN(E)
      COSNE= COS(E)
      GX1= XP(1)*COSNE  + YP(1)*SINEE
      GX2= GX1
      GY1= YP(1)*COSNE  - XP(1)*SINEE
      GY2= GY1
      DO 200 I=1,NPS
      XT= XP(I)*COSNE  + YP(I)*SINEE
      YT= YP(I)*COSNE  - XP(I)*SINEE
      IBUOY=1
      IF(VP(I).GT.90.67*(TP(I)-TA(ISCEN))*SQRT(TA(ISCEN))/TP(I)) IBUOY=0
      IRISE=2
      UINV = 1./WS(ISCEN)
      IF(HP(I).GT.10.) UINV = UINV*((10./HP(I))**P(ISC))
      EFF= 2.45*VP(I)*DP(I)*DP(I)*(TP(I)-TA(ISCEN))/TP(I)
      IPS=I
      HL(1)= HP(I)
      CALL RISE
      HL(2)= ESH(2)
      DO 170 J=1,2
      DL(J)=(BG(ISC,2)*HL(J)*HL(J)/(AG(ISC,2)*AG(ISC,2)*(BG(ISC,2)+DG(IS
     1C))))**(0.5/BG(ISC,2))*0.001
      IF(DL(J).GE.400.) GO TO 170
      DL(J)=(BG(ISC,1)*HL(J)*HL(J)/(AG(ISC,1)*AG(ISC,1)*(BG(ISC,1)+DG(IS
     1C))))**(0.5/BG(ISC,1))*0.001
  170 XTM(J)= XT + DL(J)
      IF(XTM(2).GT.GX2) GX2= XTM(2)
      IF(XTM(1).LT.GX1) GX1= XTM(1)
      IF(YT.GT.GY2)     GY2= YT
      IF(YT.LT.GY1)     GY1= YT
  200 CONTINUE
      XCRNR(1)= GX1
      XCRNR(2)= GX2
      XCRNR(3)= GX2
      XCRNR(4)= GX1
      YCRNR(1)= GY1
      YCRNR(2)= GY1
      YCRNR(3)= GY2
      YCRNR(4)= GY2
      DO 300 J=1,4
      XCRNRT= XCRNR(J)
      XCRNR(J)= XCRNR(J)*COSNE  - YCRNR(J)*SINEE
  300 YCRNR(J)= YCRNR(J)*COSNE + XCRNRT*SINEE
      XSWC= XCRNR(1)
      XNEC= XSWC
      YSWC= YCRNR(1)
      YNEC= YSWC
      DO 400 I=2,4
      IF(XCRNR(I).GT.XNEC) XNEC= XCRNR(I)
      IF(XCRNR(I).LT.XSWC) XSWC= XCRNR(I)
      IF(YCRNR(I).GT.YNEC) YNEC= YCRNR(I)
  400 IF(YCRNR(I).LT.YSWC) YSWC= YCRNR(I)
      XT= XNEC - XSWC
      YT= YNEC - YSWC
      DMAX= XT
      IF(YT.GT.XT) DMAX= YT
      IF(DMAX.LT.10.) GO TO 500
      IF(XT.GT.YT) GO TO 420
      LY=  50
      GRID= YT/50.
      LX= XT/GRID
      IF(LX.LT.50) LX= LX+1
      GO TO 600
  420 LX= 50
      GRID= XT/50.
      LY= YT/GRID
      IF(LY.LT.50) LY=LY+1
      GO TO 600
  500 IF(DMAX.LT.5.) GO TO 540
      GRID= 0.2
      LX= XT/GRID
      LY= YT/GRID
      IF(LX.LT.50) LX=LX+1
      IF(LY.LT.50) LY=LY+1
      GO TO 600
  540 IF(DMAX.LT.0.25) GO TO 580
      IF(XT.GT.YT) GO TO 560
      LY= 25
      GRID= YT/25.
      LX= XT/GRID
      IF(LX.LT.25) LX=LX+1
      GO TO 600
  560 LX= 25
      GRID= XT/25.
      LY= YT/GRID
      IF(LY.LT.25) LY=LY+1
      GO TO 600
  580 GRID= 0.01
      LX= XT/GRID
      LY= YT/GRID
      IF(LX.LT.25) LX=LX+1
      IF(LY.LT.25) LY=LY+1
  600 XSWC= XSWC - 0.5*GRID
      YSWC= YSWC - 0.5*GRID
      IF(NCSOPT.LT.1.OR.(LX.LE.25.AND.LY.LE.25)) GO TO 700
      XL=LX
      YL=LY
      IF(LX.GT.LY) GO TO 640
      DELG= YL/25.
      LY=25
      GRID= GRID*DELG
      LX= XL/DELG
      IF(LX.LT.25) LX=LX+1
      GO TO 700
  640 DELG= XL/25.
      LX=25
      GRID= GRID*DELG
      LY= YL/DELG + 1.
  700 CONTINUE
      WRITE(IWR,900)ISCEN,IWDOPT,TT
      XRSWC=XSWC+0.5*GRID
      YRSWC=YSWC+0.5*GRID
      WRITE(IWR,905)LX,LY,GRID,XRSWC,YRSWC
  900 FORMAT(1H1,'PEM:   AUTOMATICALLY GENERATED RECEPTOR GRID PARAMETER
     1S FOR SCENARIO ',I2,'  (WIND DIRECTION SUB-SCENARIO ',I2,')'//
     221X,20A4/1X,120('-')//)
  905 FORMAT(' RECEPTOR GRID CONSISTS OF ',I2,' COLUMNS AND ',I2,' ROWS
     1OF SPACING =',F7.4,' KM. SOUTHWEST CORNER OF GRID =',F8.3,' KM W,
     2',F8.3,' KM S.')
      RETURN
      END
C
C
C
      BLOCK DATA
C                 BLOCK DATA (VERSION 82360), PART OF PEM.
C
C
C
C     THIS SUBPROGRAM INITIALIZES VARIABLES IN COMMON/PEMCOM/
C
C *** PEM MODIFICATIONS BY M.M.STEVENS,
C     NOAA-ATDL, P.O.BOX-E, OAK RIDGE, TENN 37830
C     DECEMBER 1982
C
      COMMON/PEMCOM/CONC(50,50,2),SDF(50,50,2),  TT(20),
     1 XP(300),YP(300),EP(300,2),HP(300),DP(300),VP(300),TP(300),
     2 XA(50),YA(50),EA(50,2),SIZE(50),
     3 WD(24),WS(24),TA(24),HMIX(24),PEN(24),
     4 AX(7,3),BX(7,3),P(7),SCLAB(7),DTDZ(2),  SECTAN(16),
     5 XSWC,YSWC,GRID,LX,LY,    A(2),B(2),POLNAM(3,2),CALNAM(7,2),
     6 ITA,IRD,IWR,IDSK,        D80,D47,D8047,DIST,DELTA,
     7 ESH(2),PEAK,IBUOY,IRISE,IDWN,EFF,XS,    UINV,WVEC,
     8 NAS,NPS,INDEX,IGRID,IAV,ISCEN,IWDOPT,IWD,ISC,IPS,
     9 NTOPT,NWDOPT,NWSOPT,NSCEN,NLIST,NARRAY,NTAPE,NCSOPT,NMAX,
     * NSTDWN,INTER,NPRINT
C
C
      DATA INDEX,NAS,NPS/0,0,0/
      DATA ITA,IRD,IWR,IDSK/1,5,6,8/
      DATA SCLAB/2HA ,2HB ,2HC ,2HDD,2HDN,2HE ,2HF /
      DATA P/0.1,0.15,0.2,0.25,0.25,0.3,0.3/
      DATA AX/.0383,.1393,.112,.0856,.0818,.1094,.05645,
     1 .0002539,.04936,.1014,.2591,.2527,.2452,.1930,
     2 .0002539,.04936,.1154,.7368,1.297,.9204,1.505/
      DATA BX/1.281,.9467,.9100,.865,.8155,.7657,.805,
     1  2.089,1.114,.926,.6869,.6341,.6358,.6072,
     2 2.089,1.114,.9109,.5642,.4421,.4805,.3662/
      DATA SECTAN/0.,.39270,.78540,1.17810,1.57080,1.96350,2.35620,
     1 2.74890,3.14159,3.53429,3.92699,4.31969,4.71239,5.10509,
     2 5.49779,5.89049/
C
      END
C
C
C
      SUBROUTINE D01AJF(F, A, B, EPSABS, EPSREL, RESULT, ABSERR,WORK,
     * LWORK, IWORK, LIWORK, IFAIL)
C                    SUBROUTINE D01AJF, PART OF PEM (VERSION 82360).
C
C     MARK 8 RELEASE. NAG COPYRIGHT 1980
C
C     D01AJF IS A GENERAL PURPOSE INTEGRATOR WHICH CALCULATES
C     AN APPROXIMATION TO THE INTEGRAL OF A FUNCTION OVER A FINITE
C     INTERVAL (A,B).  THIS ROUTINE CAN BE USED WHEN THE INTEGRAND
C     HAS SINGULARITIES, ESPECIALLY WHEN THESE ARE OF ALGEBRAIC OR
C     LOGARITHMIC TYPE.  D01AJF IS AN ADAPTIVE ROUTINE, USING THE
C     GAUSS 10-POINT AND KRONROD 21-POINT RULES.  THE ALGORITHM
C     INCORPORATES A GLOBAL ACCEPTANCE CRITERION TOGETHER WITH
C     EPS-ALGORITHM TO PERFORM EXTRAPOLATION.  THE LOCAL ERROR IS
C     ESTIMATED.
C
C     THE GENERAL PURPOSE INTEGRATOR D01AJF INCLUDES THE FOLLOWING:
C     SUBROUTINES (1) D01AJF, (2) D01AJV, (3) D01AJX, (4) D01AJY,
C     (5) D01AJZ, INTEGER FUNCTION P01AAF, DOUBLE PRECISION FUNCTIONS
C     (1) X02AAF, (2) X02ABF, (3) X02ACF, AND SUBROUTINE X04AAF.
C     THE PROGRAM LISTINGS FOR THESE SUBROUTINES AND FUNCTIONS, COPIED
C     HERE FROM ORNL - NAG LIBRARY, FOLLOW.  THESE ARE DEVELOPED BY
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C     WHICH HOLDS THE COPYRIGHT (NAG FORTRAN MINI MANUAL, MARK8, 1980).
C     THESE PROGRAM LISTINGS ARE INCLUDED HERE WITH PERMISSION FROM
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C     EXCLUSIVELY FOR PEM.  THESE LIBRARY SUBROUTINES AND PROGRAMS
C     SHOULD NOT BE USED FOR ANY OTHER PURPOSE WITHOUT PRIOR APPROVAL
C     FROM NAG AND ORNL.
C
C
C     D01AJF ITSELF IS ESSENTIALLY A DUMMY ROUTINE WHOSE FUNCTION IS TO
C     PARTITION THE WORK ARRAYS WORK AND IWORK FOR USE BY D01AJV.
C     WORK IS PARTITIONED INTO 4 ARRAYS EACH OF SIZE LWORK/4.
C     IWORK IS A SINGLE ARRAY IN D01AJV.
C
C     .. SCALAR ARGUMENTS ..
      DOUBLE PRECISION A, ABSERR, B, EPSABS, EPSREL, RESULT
      INTEGER IFAIL, LIWORK, LWORK
C     .. ARRAY ARGUMENTS ..
      DOUBLE PRECISION WORK(LWORK)
      INTEGER IWORK(LIWORK)
C     .. FUNCTION ARGUMENTS ..
      DOUBLE PRECISION F
C     ..
C     .. LOCAL SCALARS ..
C$P 1
      DOUBLE PRECISION SRNAME
      INTEGER IBL, IEL, IER, IRL, LIMIT
C     .. FUNCTION REFERENCES ..
```

```
      INTEGER P01AAF                                                    00033840
C     .. SUBROUTINE REFERENCES ..                                       00033850
C     D01AJV                                                            00033860
C     ..                                                                00033870
      EXTERNAL F                                                        00033880
      DATA SRNAME /8H D01AJF /                                          00033890
C     CHECK THAT MINIMUM WORKSPACE REQUIREMENTS ARE MET                 00033900
      IF (LWORK.LT.4) GO TO 20                                          00033910
      IF (LIWORK.LT.LWORK/8+2) GO TO 20                                 00033920
C     LIMIT = UPPER BOUND ON NUMBER OF SUBINTERVALS                     00033930
      LIMIT = LWORK/4                                                   00033940
C     SET UP BASE ADDRESSES FOR WORK ARRAYS                             00033950
      IBL = LIMIT + 1                                                   00033960
      IEL = LIMIT + IBL                                                 00033970
      IRL = LIMIT + IEL                                                 00033980
C     PERFORM INTEGRATION                                               00033990
      CALL D01AJV(F, A, B, DABS(EPSABS), DABS(EPSREL), WORK(1),WORK(IBL)00034000
     *, WORK(IEL), WORK(IRL), LIMIT, IWORK, LIWORK,RESULT, ABSERR, IER) 00034010
      IF (IER.NE.0) GO TO 40                                            00034020
      IFAIL = 0                                                         00034030
      GO TO 60                                                          00034040
C     ERROR 6 = INSUFFICIENT WORKSPACE                                  00034050
   20 IER = 6                                                           00034060
   40 IFAIL = P01AAF(IFAIL,IER,SRNAME)                                  00034070
   60 RETURN                                                            00034080
      END                                                               00034090
C                                                                       00034100
C                                                                       00034110
      SUBROUTINE D01AJV(F, A, B, EPSABS, EPSREL, ALIST, BLIST,ELIST,    00034120
     * RLIST, LIMIT, IORD, LIORD, RESULT, ABSERR, IER)                  00034130
C                      SUBROUTINE D01AJV, PART OF PEM (VERSION 82360).  00034140
C                                                                       00034150
C     MARK 8 RELEASE. NAG COPYRIGHT 1979                                00034160
C     BASED ON QUADPACK ROUTINE DQAGS (FORMERLY QAGS)                   00034170
C     ***********************************************************       00034180
C                                                                       00034190
C        PURPOSE                                                        00034200
C           THE ROUTINE CALCULATES AN APPROXIMATION                     00034210
C           /RESULT/ TO A GIVEN DEFINITE INTEGRAL   I =                 00034220
C           INTEGRAL OF /F/ OVER (A,B), HOPEFULLY                       00034230
C           SATISFYING FOLLOWING CLAIM FOR ACCURACY .                   00034240
C           ABS(I-RESULT) .LE. MAX(EPSABS,EPSREL*ABS(I)).               00034250
C                                                                       00034260
C          CALLING SEQUENCE                                             00034270
C           CALL D01AJV (F,A,B,EPSABS,EPSREL,ALIST,BLIST,ELIST,         00034280
C                        RLIST,LIMIT,IORD,LIORD,RESULT,ABSERR,IER)      00034290
C                                                                       00034300
C        PARAMETERS                                                     00034310
C            F      - FUNCTION SUBPROGRAM DEFINING THE INTEGRAND        00034320
C                     FUNCTION F(X). THE ACTUAL NAME FOR F              00034330
C                     NEEDS TO BE DECLARED E X T E R N A L              00034340
C                     IN THE DRIVER PROGRAM                             00034350
C                                                                       00034360
C            A      - LOWER LIMIT OF INTEGRATION                        00034370
C                                                                       00034380
C            B      - UPPER LIMIT OF INTEGRATION                        00034390
C                                                                       00034400
C            EPSABS - ABSOLUTE ACCURACY REQUESTED                       00034410
C                                                                       00034420
C            EPSREL - RELATIVE ACCURACY REQUESTED                       00034430
C                                                                       00034440
C            ALIST,BLIST,ELIST,RLIST                                    00034450
C                   - WORK ARRAYS (FUNCTIONS DESCRIBED BELOW)           00034460
C                                                                       00034470
C            LIMIT  - UPPER BOUND FOR NUMBER OF SUBINTERVALS            00034480
C                                                                       00034490
C            IORD   - WORK ARRAY                                        00034500
C                                                                       00034510
C            LIORD  - LENGTH OF IORD (AT LEAST LIMIT/2 + 2)             00034520
C                                                                       00034530
C            RESULT - APPROXIMATION TO THE INTEGRAL                     00034540
C                                                                       00034550
C            ABSERR - ESTIMATE OF THE MODULUS OF THE ABSOLUTE ERROR,    00034560
C                     WHICH SHOULD EQUAL OR EXCEED ABS(I-RESULT)        00034570
C                                                                       00034580
C            IER    - IER    = 0 NORMAL AND RELIABLE                    00034590
C                              TERMINATION OF THE ROUTINE.              00034600
```

```
C                                 IT IS ASSUMED THAT THE                  00034610
C                                 REQUESTED  ACCURACY HAS BEEN            00034620
C                                 ACHIEVED.                               00034630
C                    - IER   .NE. 0 ABNORMAL TERMINATION OF               00034640
C                                 THE ROUTINE. THE ESTIMATES              00034650
C                                 FOR INTEGRAL AND ERROR ARE              00034660
C                                 LESS RELIABLE. IT IS ASSUMED            00034670
C                                 THAT THE  REQUESTED ACCURACY            00034680
C                                 HAS NOT BEEN ACHIEVED.                  00034690
C                           = 1 MAXIMUM NUMBER OF SUBDIVISIONS ALLOWED    00034700
C                                 HAS BEEN ACHIEVED. THE USER CAN         00034710
C                                 ALLOW MORE SUB DIVISIONS BY             00034720
C                                 INCREASING THE DIMENSIONS OF THE        00034730
C                                 WORK ARRAYS WORK AND IWORK.             00034740
C                                 HOWEVER, THIS MAY                       00034750
C                                 YIELD NO  IMPROVEMENT, AND IT           00034760
C                                 IS RATHER ADVISED TO HAVE A             00034770
C                                 CLOSE LOOK AT THE INTEGRAND,            00034780
C                                 IN ORDER TO DETERMINE THE               00034790
C                                 INTEGRATION  DIFFICULTIES. IF           00034800
C                                 THE POSITION OF A LOCAL                 00034810
C                                 DIFFICULTY CAN BE DETERMINED            00034820
C                                 (I.E.  SINGULARITY,                     00034830
C                                 DISCONTINUITY WITHIN THE                00034840
C                                 INTERVAL) ONE WILL PROBABLY             00034850
C                                 GAIN FROM  SPLITTING UP THE             00034860
C                                 INTERVAL AT THIS POINT AND              00034870
C                                 CALLING THE INTEGRATOR ON THE           00034880
C                                 SUB-RANGES. IF POSSIBLE, AN             00034890
C                                 APPROPRIATE SPECIAL-PURPOSE             00034900
C                                 INTEGRATOR SHOULD BE USED               00034910
C                                 WHICH IS DESIGNED FOR                   00034920
C                                 HANDLING THE TYPE  OF                   00034930
C                                 DIFFICULTY INVOLVED.                    00034940
C                           = 2 THE OCCURRENCE OF ROUNDOFF                00034950
C                                 ERROR IS DETECTED WHICH                 00034960
C                                 PREVENTS THE REQUESTED                  00034970
C                                 TOLERANCE  FROM BEING                   00034980
C                                 ACHIEVED. THE ERROR MAY BE              00034990
C                                 UNDER-ESTIMATED.                        00035000
C                           = 3 EXTREMELY BAD INTEGRAND BEHAVIOUR         00035010
C                                 OCCURS AT SOME INTERIOR POINTS OF THE   00035020
C                                 INTEGRATION INTERVAL.                   00035030
C                           = 4 IT IS PRESUMED THAT THE REQUESTED         00035040
C                                 TOLERANCE CANNOT BE ACHIEVED,           00035050
C                                 AND THAT THE RETURNED RESULT            00035060
C                                 IS THE BEST WHICH CAN BE                00035070
C                                 OBTAINED.                               00035080
C                           = 5 THE INTEGRAL IS PROBABLY DIVERGENT, OR    00035090
C                                 SLOWLY CONVERGENT. IT MUST BE NOTED     00035100
C                                 THAT DIVERGENCY CAN OCCUR               00035110
C                                 WITH ANY OTHER VALUE OF IER.            00035120
C                                                                         00035130
C     ***********************************************************         00035140
C     .. SCALAR ARGUMENTS ..                                              00035150
      DOUBLE PRECISION A, ABSERR, B, EPSABS, EPSREL, RESULT               00035160
      INTEGER IER, LIMIT, LIORD                                           00035170
C     .. ARRAY ARGUMENTS ..                                               00035180
      DOUBLE PRECISION ALIST(LIMIT), BLIST(LIMIT), ELIST(LIMIT),          00035190
     * RLIST(LIMIT)                                                       00035200
      INTEGER IORD(LIORD)                                                 00035210
C     .. FUNCTION ARGUMENTS ..                                            00035220
      DOUBLE PRECISION F                                                  00035230
C     ..                                                                  00035240
C     .. SCALARS IN COMMON ..                                             00035250
      INTEGER JUPBND                                                      00035260
C     ..                                                                  00035270
C     .. LOCAL SCALARS ..                                                 00035280
      DOUBLE PRECISION A1, A2, ABSEPS, AREA12, AREA1, AREA2, AREA, B1,    00035290
     * B2,CORREC, DEFAB1, DEFAB2, DEFABS, DRES, EPMACH, ERLARG,ERLAST,     00035300
     * ERRBND, ERRMAX, ERRO12, ERROR1, ERROR2, ERRSUM,ERTEST, OFLOW,      00035310
     * RESABS, RESEPS, SMALL, UFLOW                                       00035320
      INTEGER ID, IERRO, IROFF1, IROFF2, IROFF3, K, KSGN, KTMIN,LAST1,    00035330
     * LAST, MAXERR, NRES, NRMAX, NUMRL2                                  00035340
      LOGICAL EXTRAP, NOEXT                                               00035350
C     .. LOCAL ARRAYS ..                                                  00035360
      DOUBLE PRECISION RES3LA(3), RLIST2(52)                              00035370
```

```
C     .. FUNCTION REFERENCES ..
      DOUBLE PRECISION X02AAF, X02ABF, X02ACF
C     .. SUBROUTINE REFERENCES ..
C     D01AJX, D01AJY, D01AJZ
C     ..
      EXTERNAL F
      COMMON /AD01AJ/ JUPBND
C
C            THE DIMENSION OF /RLIST2/ IS DETERMINED BY
C            DATA /LIMEXP/ IN SUBROUTINE D01AJY (/RLIST2/
C            SHOULD BE OF DIMENSION (LIMEXP+2) AT LEAST).
C
      EPMACH = X02AAF(1.0D0)
      UFLOW = X02ABF(1.0D0)
      OFLOW = X02ACF(1.0D0)
C
C            LIST OF MAJOR VARIABLES
C            -----------------------
C
C           ALIST     - LIST OF LEFT END-POINTS OF ALL SUBINTERVALS
C                       CONSIDERED UP TO NOW
C
C           BLIST     - LIST OF RIGHT END-POINTS OF ALL SUBINTERVALS
C                       CONSIDERED UP TO NOW
C
C           RLIST(I)  - APPROXIMATION TO THE INTEGRAL OVER
C                       (ALIST(I),BLIST(I))
C
C           RLIST2    - ARRAY OF DIMENSION AT LEAST LIMEXP+2
C                       CONTAINING THE PART OF THE EPSILON TABLE
C                       WHICH IS STILL NEEDED FOR FURTHER
C                       COMPUTATIONS
C
C           ELIST(I)  - ERROR ESTIMATE APPLYING TO RLIST(I)
C
C           MAXERR    - POINTER TO THE INTERVAL WITH LARGEST ERROR
C                       ESTIMATE
C
C           ERRMAX    - ELIST(MAXERR)
C
C           ERLAST    - ERROR ON THE INTERVAL CURRENTLY SUBDIVIDED
C                       (BEFORE THAT SUBDIVISION HAS TAKEN PLACE)
C
C           AREA      - SUM OF THE INTEGRALS OVER THE SUBINTERVALS
C
C           ERRSUM    - SUM OF THE ERRORS OVER THE SUBINTERVALS
C
C           ERRBND    - REQUESTED ACCURACY MAX(EPSABS,EPSREL*
C                       ABS(RESULT))
C
C           *****1    - VARIABLE FOR THE LEFT INTERVAL
C
C           *****2    - VARIABLE FOR THE RIGHT INTERVAL
C
C           LAST      - INDEX FOR SUBDIVISION
C
C           NRES      - NUMBER OF CALLS TO THE EXTRAPOLATION ROUTINE
C
C           NUMRL2    - NUMBER OF ELEMENTS CURRENTLY  IN
C                       RLIST2. IF AN APPROPRIATE
C                       APPROXIMATION TO THE COMPOUNDED
C                       INTEGRAL HAS BEEN OBTAINED IT IS
C                       PUT IN  RLIST2(NUMRL2) AFTER NUMRL2
C                       HAS BEEN INCREASED BY ONE.
C
C           SMALL     - LENGTH OF THE SMALLEST INTERVAL CONSIDERED
C                       UP TO NOW, MULTIPLIED BY 1.5
C
C           ERLARG    - SUM OF THE ERRORS OVER THE INTERVALS LARGER
C                       THAN THE SMALLEST INTERVAL
C                       CONSIDERED UP TO NOW
C           EXTRAP    - LOGICAL VARIABLE DENOTING THAT THE
C                       ROUTINE IS ATTEMPTING TO PERFORM
C                       EXTRAPOLATION.  I.E. BEFORE
C                       SUBDIVIDING THE SMALLEST INTERVAL
C                       WE TRY TO DECREASE THE VALUE OF
C                       ERLARG
```

```
C           NOEXT     - LOGICAL VARIABLE DENOTING THAT EXTRAPOLATION
C                       IS NO LONGER ALLOWED(/TRUE/ VALUE)
C
C           FIRST APPROXIMATION TO THE INTEGRAL
C           -----------------------------------
C
      LAST1 = 1
      IER = 0
      IERRO = 0
      CALL D01AJZ(F, A, B, RESULT, ABSERR, DEFABS, RESABS)
C
C           TEST ON ACCURACY
C
      DRES = DABS(RESULT)
      ERRBND = DMAX1(EPSABS,EPSREL*DRES)
      IF (ABSERR.LE.1.0D+02*EPMACH*DEFABS .AND. ABSERR.GT.ERRBND)IER = 2
      IF (LIMIT.LT.2 .AND. ABSERR.GT.ERRBND) IER = 1
      IF (IER.NE.0 .OR. ABSERR.LE.ERRBND) GO TO 320
C
C           INITIALIZATION
C           --------------
C
      ALIST(1) = A
      BLIST(1) = B
      RLIST(1) = RESULT
      RLIST2(1) = RESULT
      ERRMAX = ABSERR
      MAXERR = 1
      AREA = RESULT
      ERRSUM = ABSERR
      ABSERR = OFLOW
      NRMAX = 1
      NRES = 0
      NUMRL2 = 2
      KTMIN = 0
      EXTRAP = .FALSE.
      NOEXT = .FALSE.
      IROFF1 = 0
      IROFF2 = 0
      IROFF3 = 0
      KSGN = -1
      IF (DRES.GE.(0.1D+01-0.5D+02*EPMACH)*DEFABS) KSGN = 1
C
C           MAIN DO-LOOP
C           ------------
C
      IF (LIMIT.LT.2) GO TO 220
      DO 200 LAST=2,LIMIT
C
C           BISECT THE SUBINTERVAL WITH THE NRMAX-TH LARGEST
C           ERROR ESTIMATE
C
        LAST1 = LAST
        A1 = ALIST(MAXERR)
        B1 = 0.5D+00*(ALIST(MAXERR)+BLIST(MAXERR))
        A2 = B1
        B2 = BLIST(MAXERR)
        ERLAST = ERRMAX
        CALL D01AJZ(F, A1, B1, AREA1, ERROR1, RESABS, DEFAB1)
        CALL D01AJZ(F, A2, B2, AREA2, ERROR2, RESABS, DEFAB2)
C
C           IMPROVE PREVIOUS APPROXIMATION OF INTEGRAL
C           AND ERROR AND TEST FOR ACCURACY
C
        AREA12 = AREA1 + AREA2
        ERRO12 = ERROR1 + ERROR2
        ERRSUM = ERRSUM + ERRO12 - ERRMAX
        AREA = AREA + AREA12 - RLIST(MAXERR)
        IF (DEFAB1.EQ.ERROR1 .OR. DEFAB2.EQ.ERROR2) GO TO 40
        IF (DABS(RLIST(MAXERR)-AREA12).GT.0.1D-04*DABS(AREA12) .OR.
     *  ERRO12.LT.0.99D+00*ERRMAX) GO TO 20
        IF (EXTRAP) IROFF2 = IROFF2 + 1
        IF (.NOT.EXTRAP) IROFF1 = IROFF1 + 1
   20   IF (LAST.GT.10 .AND. ERRO12.GT.ERRMAX) IROFF3 = IROFF3 + 1
   40   RLIST(MAXERR) = AREA1
        RLIST(LAST) = AREA2
        ERRBND = DMAX1(EPSABS,EPSREL*DABS(AREA))
      IF (ERRSUM.LE.ERRBND) GO TO 280                                   00036920
C                                                                       00036930
C         TEST FOR ROUNDOFF ERROR AND EVENTUALLY                        00036940
C         SET ERROR FLAG                                                00036950
C                                                                       00036960
      IF (IROFF1+IROFF2.GE.10 .OR. IROFF3.GE.20) IER = 2                00036970
      IF (IROFF2.GE.5) IERRO = 3                                        00036980
C                                                                       00036990
C         SET ERROR FLAG IN THE CASE THAT THE NUMBER OF INTERVAL        00037000
C          BISECTIONS EXCEEDS /LIMIT/                                   00037010
C                                                                       00037020
      IF (LAST.EQ.LIMIT) IER = 1                                        00037030
C                                                                       00037040
C         SET ERROR FLAG IN THE CASE OF BAD INTEGRAND BEHAVIOUR         00037050
C         AT INTERIOR POINTS OF INTEGRATION RANGE                       00037060
C                                                                       00037070
      IF (DMAX1(DABS(A1),DABS(B2)).LE.(0.1D+01+0.1D+03*EPMACH)*         00037080
     * (DABS(A2)+0.1D+04*UFLOW)) IER = 4                                00037090
      IF (IER.NE.0) GO TO 220                                           00037100
C                                                                       00037110
C         APPEND THE NEWLY-CREATED INTERVALS TO THE LIST                00037120
C                                                                       00037130
      IF (ERROR2.GT.ERROR1) GO TO 60                                    00037140
      ALIST(LAST) = A2                                                  00037150
      BLIST(MAXERR) = B1                                                00037160
      BLIST(LAST) = B2                                                  00037170
      ELIST(MAXERR) = ERROR1                                            00037180
      ELIST(LAST) = ERROR2                                              00037190
      GO TO 80                                                          00037200
   60 ALIST(MAXERR) = A2                                                00037210
      ALIST(LAST) = A1                                                  00037220
      BLIST(LAST) = B1                                                  00037230
      RLIST(MAXERR) = AREA2                                             00037240
      RLIST(LAST) = AREA1                                               00037250
      ELIST(MAXERR) = ERROR2                                            00037260
      ELIST(LAST) = ERROR1                                              00037270
C                                                                       00037280
C         CALL SUBROUTINE D01AJX TO MAINTAIN THE                        00037290
C         DESCENDING ORDERING IN THE LIST OF ERROR                      00037300
C         ESTIMATES AND SELECT THE SUBINTERVAL WITH                     00037310
C         NRMAX-TH LARGEST ERROR ESTIMATE (TO BE BISECTED               00037320
C         NEXT)                                                         00037330
C                                                                       00037340
   80 CALL D01AJX(LIMIT, LAST, MAXERR, ERRMAX, ELIST, IORD,LIORD,       00037350
     *  NRMAX)                                                          00037360
      IF (LAST.EQ.2) GO TO 180                                          00037370
      IF (NOEXT) GO TO 200                                              00037380
      ERLARG = ERLARG - ERLAST                                          00037390
      IF (DABS(B1-A1).GT.SMALL) ERLARG = ERLARG + ERRO12                00037400
      IF (EXTRAP) GO TO 100                                             00037410
C                                                                       00037420
C         TEST WHETHER THE INTERVAL TO BE BISECTED NEXT IS THE          00037430
C         SMALLEST INTERVAL                                             00037440
C                                                                       00037450
      IF (DABS(BLIST(MAXERR)-ALIST(MAXERR)).GT.SMALL) GO TO 200         00037460
      EXTRAP = .TRUE.                                                   00037470
      NRMAX = 2                                                         00037480
  100 IF (IERRO.EQ.3 .OR. ERLARG.LE.ERTEST) GO TO 140                   00037490
C                                                                       00037500
C         THE SMALLEST INTERVAL HAS THE LARGEST ERROR.                  00037510
C         BEFORE BISECTING DECREASE THE SUM OF THE ERRORS               00037520
C         OVER THE LARGER INTERVALS(ERLARG) AND PERFORM                 00037530
C         EXTRAPOLATION                                                 00037540
C                                                                       00037550
      ID = NRMAX                                                        00037560
      DO 120 K=ID,JUPBND                                                00037570
         MAXERR = IORD(NRMAX)                                           00037580
         ERRMAX = ELIST(MAXERR)                                         00037590
         IF (DABS(BLIST(MAXERR)-ALIST(MAXERR)).GT.SMALL) GO TO 200      00037600
         NRMAX = NRMAX + 1                                              00037610
  120 CONTINUE                                                          00037620
C                                                                       00037630
C         PERFORM EXTRAPOLATION                                         00037640
C                                                                       00037650
  140 NUMRL2 = NUMRL2 + 1                                               00037660
      RLIST2(NUMRL2) = AREA                                             00037670
      CALL D01AJY(NUMRL2, RLIST2, RESEPS, ABSEPS, RES3LA, NRES)         00037680
```

```
          KTMIN = KTMIN + 1
          IF (KTMIN.GT.5 .AND. ABSERR.LT.0.1D-02*ERRSUM) IER = 5
          IF (ABSEPS.GE.ABSERR) GO TO 160
          KTMIN = 0
          ABSERR = ABSEPS
          RESULT = RESEPS
          CORREC = ERLARG
          ERTEST = DMAX1(EPSABS,EPSREL*DABS(RESEPS))
          IF (ABSERR.LE.ERTEST) GO TO 220
C
C           PREPARE  BISECTION OF THE SMALLEST INTERVAL
C
  160     IF (NUMRL2.EQ.1) NOEXT = .TRUE.
          IF (IER.EQ.5) GO TO 220
          MAXERR = IORD(1)
          ERRMAX = ELIST(MAXERR)
          NRMAX = 1
          EXTRAP = .FALSE.
          SMALL = SMALL*0.5D+00
          ERLARG = ERRSUM
          GO TO 200
  180     SMALL = DABS(B-A)*0.375D+00
          ERLARG = ERRSUM
          ERTEST = ERRBND
          RLIST2(2) = AREA
  200 CONTINUE
C
C           SET  FINAL RESULT AND ERROR ESTIMATE
C           ------------------------------------
C
  220 IF (ABSERR.EQ.OFLOW) GO TO 280
      IF (IER+IERRO.EQ.0) GO TO 260
      IF (IERRO.EQ.3) ABSERR = ABSERR + CORREC
      IF (IER.EQ.0) IER = 3
      IF (RESULT.NE.0.D+00.AND .AREA. NE.0.D+00) GO TO 240
      IF (ABSERR.GT.ERRSUM) GO TO 280
      IF (AREA.EQ.0.D+00) GO TO 320
      GO TO 260
  240 IF (ABSERR/DABS(RESULT).GT.ERRSUM/DABS(AREA)) GO TO 280
C
C           TEST ON DIVERGENCY
C
  260 IF (KSGN.EQ.-1 .AND. DMAX1(DABS(RESULT),DABS(AREA)).LE.DEFABS*
     *0.1D-01) GO TO 320
      IF (0.1D-01.GT.(RESULT/AREA) .OR. (RESULT/AREA).GT.0.1D+03.OR.
     * ERRSUM.GT.DABS(AREA)) IER = 6
      GO TO 320
C
C           COMPUTE GLOBAL INTEGRAL SUM
C
  280 RESULT = 0.D+00
      DO 300 K=1,LAST
         RESULT = RESULT + RLIST(K)
  300 CONTINUE
      ABSERR = ERRSUM
  320 IF (IER.GT.2) IER = IER - 1
      IORD(1) = 4*LAST1
      RETURN
      END
C
C
      SUBROUTINE D01AJX(LIMIT, LAST, MAXERR, ERMAX, ELIST, IORD,LIORD,
     * NRMAX)
C
C                    SUBROUTINE D01AJX, PART OF PEM (VERSION 82360).
C
C     MARK 8 RELEASE. NAG COPYRIGHT 1979
C     BASED ON QUADPACK ROUTINE ORDER
C     ***************************************************
C
C           PURPOSE
C              THIS ROUTINE MAINTAINS THE DESCENDING ORDERING
C              IN THE LIST OF THE LOCAL ERROR ESTIMATES
C              RESULTING FROM THE INTERVAL SUBDIVISION
C              PROCESS. AT EACH CALL TWO ERROR ESTIMATES
C              ARE INSERTED USING THE SEQUENTIAL SEARCH
C              METHOD . TOP-DOWN FOR THE LARGEST ERROR
C              ESTIMATE,  BOTTOM-UP FOR THE SMALLEST ERROR
```

```
C                 ESTIMATE.
C
C            CALLING SEQUENCE
C               CALL D01AJX
C               (LIMIT,LAST,MAXERR,ERMAX,ELIST,IORD,LIORD,NRMAX)
C
C              PARAMETERS (MEANING AT OUTPUT)
C               LIMIT  - MAXIMUM NUMBER OF ERROR ESTIMATES THE LIST
C                        CAN CONTAIN
C
C               LAST   - NUMBER OF ERROR ESTIMATES CURRENTLY
C                        IN THE LIST. ELIST(LAST) CONTAINS
C                        THE SMALLEST ERROR ESTIMATE.
C
C               MAXERR - MAXERR POINTS TO THE NRMAX-TH LARGEST ERROR
C                        ESTIMATE CURRENTLY IN THE LIST.
C
C               ERMAX  - NRMAX-TH LARGEST ERROR ESTIMATE
C                        ERMAX = ELIST(MAXERR)
C
C               ELIST  - ARRAY OF DIMENSION LAST CONTAINING
C                        THE ERROR ESTIMATES
C
C               IORD   - ARRAY CONTAINING POINTERS TO ELIST SO
C                        THAT IORD(1) POINTS TO THE LARGEST
C                        ERROR ESTIMATE,...,IORD(LAST) TO THE
C                        SMALLEST ERROR ESTIMATE
C
C               LIORD  - DIMENSION OF IORD
C
C               NRMAX  - MAXERR = IORD(NRMAX)
C
C     ****************************************************
C
C     .. SCALAR ARGUMENTS ..
      DOUBLE PRECISION ERMAX
      INTEGER LAST, LIMIT, LIORD, MAXERR, NRMAX
C     .. ARRAY ARGUMENTS ..
      DOUBLE PRECISION ELIST(LAST)
      INTEGER IORD(LIORD)
C     ..
C     .. SCALARS IN COMMON ..
      INTEGER JUPBND
C     ..
C     .. LOCAL SCALARS ..
      DOUBLE PRECISION ERRMAX, ERRMIN
      INTEGER I, IBEG, IDO, ISUCC, J, JBND, K
C     ..
      COMMON /AD01AJ/ JUPBND
C
C            CHECK WHETHER THE LIST CONTAINS MORE THAN
C            TWO ERROR ESTIMATES
C
      IF (LAST.GT.2) GO TO 20
      IORD(1) = 1
      IORD(2) = 2
      GO TO 180
C
C            THIS PART OF THE ROUTINE IS ONLY EXECUTED
C            IF, DUE TO A DIFFICULT INTEGRAND, SUBDIVISION
C            INCREASED THE ERROR ESTIMATE. IN THE NORMAL CASE
C            THE INSERT PROCEDURE SHOULD START AFTER THE
C            NRMAX-TH LARGEST ERROR ESTIMATE.
C
   20 ERRMAX = ELIST(MAXERR)
      IF (NRMAX.EQ.1) GO TO 60
      IDO = NRMAX - 1
      DO 40 I=1,IDO
         ISUCC = IORD(NRMAX-1)
         IF (ERRMAX.LE.ELIST(ISUCC)) GO TO 60
         IORD(NRMAX) = ISUCC
         NRMAX = NRMAX - 1
   40 CONTINUE
C
C            COMPUTE THE NUMBER OF ELEMENTS IN THE LIST TO
C            BE MAINTAINED IN DESCENDING ORDER. THIS NUMBER
C            DEPENDS ON THE NUMBER OF SUBDIVISIONS STILL
```

```
C           ALLOWED
C
   60 JUPBND = LAST
      IF (LAST.GT.(LIMIT/2+2)) JUPBND = LIMIT + 3 - LAST
      ERRMIN = ELIST(LAST)
C
C           INSERT ERRMAX BY TRAVERSING THE LIST TOP-DOWN
C           STARTING COMPARISON FROM THE ELEMENT
C           ELIST(IORD(NRMAX+1))
C
      JBND = JUPBND - 1
      IBEG = NRMAX + 1
      IF (IBEG.GT.JBND) GO TO 100
      DO 80 I=IBEG,JBND
         ISUCC = IORD(I)
         IF (ERRMAX.GE.ELIST(ISUCC)) GO TO 120
         IORD(I-1) = ISUCC
   80 CONTINUE
  100 IORD(JBND) = MAXERR
      IORD(JUPBND) = LAST
      GO TO 180
C
C           INSEPT ERRMIN BY TRAVERSING THE LIST BOTTOM-UP
C
  120 IORD(I-1) = MAXERR
      K = JBND
      DO 140 J=I,JBND
         ISUCC = IORD(K)
         IF (ERRMIN.LT.ELIST(ISUCC)) GO TO 160
         IORD(K+1) = ISUCC
         K = K - 1
  140 CONTINUE
      IORD(I) = LAST
      GO TO 180
  160 IORD(K+1) = LAST
C
C           SET MAXERR AND ERMAX
C
  180 MAXERR = IORD(NRMAX)
      ERMAX = ELIST(MAXERR)
      RETURN
      END
C
C
      SUBROUTINE D01AJY(N, EPSTAB, RESULT, ABSERR, RES3LA, NRES)
C                     SUBROUTINE D01AJY, PART OF PEM (VERSION 82360).
C     MARK 8 RELEASE. NAG COPYRIGHT 1979
C     BASED ON QUADPACK ROUTINE EPSALG
C     **************************************************
C
C           PURPOSE
C              THE ROUTINE TRANSFORMS A GIVEN SEQUENCE OF
C              APPROXIMATIONS, BY MEANS OF THE EPSILON
C              ALGORITHM OF P. WYNN.
C
C              AN ESTIMATE OF THE ABSOLUTE ERROR IS ALSO GIVEN.
C              THE CONDENSED EPSILON TABLE IS COMPUTED. ONLY THOSE
C              ELEMENTS NEEDED FOR THE COMPUTATION OF THE
C              NEXT DIAGONAL ARE PRESERVED.
C
C           CALLING SEQUENCE
C              CALL D01AJY (N,EPSTAB,RESULT,ABSERR,RES3LA,NRES)
C
C           PARAMETERS
C              N      - EPSTAB(N) CONTAINS THE NEW ELEMENT IN THE
C                       FIRST COLUMN OF THE EPSILON TABLE.
C
C              EPSTAB - ONE DIMENSIONAL ARRAY CONTAINING THE
C                       ELEMENTS OF THE TWO LOWER DIAGONALS OF
C                       THE TRIANGULAR EPSILON TABLE.
C                       THE ELEMENTS ARE NUMBERED STARTING AT THE
C                       RIGHT-HAND CORNER OF THE TRIANGLE.
C                       THE DIMENSION SHOULD BE AT LEAST N+2.
C
C              RESULT - RESULTING APPROXIMATION TO THE INTEGRAL
```

```
C              ABSERR - ESTIMATE OF THE ABSOLUTE ERROR COMPUTED FROM
C                       RESULT AND THE 3 PREVIOUS /RESULTS/
C
C              RES3LA - ARRAY CONTAINING THE LAST 3 /RESULTS/
C
C              NRES   - NUMBER OF CALLS TO THE ROUTINE
C                       (SHOULD BE ZERO AT FIRST CALL)
C
C     **************************************************
C     .. SCALAR ARGUMENTS ..
      DOUBLE PRECISION ABSERR, RESULT
      INTEGER N, NRES
C     .. ARRAY ARGUMENTS ..
      DOUBLE PRECISION EPSTAB(52), RES3LA(3)
C     ..
C     .. LOCAL SCALARS ..
      DOUBLE PRECISION DELTA1, DELTA2, DELTA3, E0, E1, E1ABS, E2, E3,
     * EPMACH,EPSINF, ERR1, ERR2, ERR3, ERROR, OFLOW, RES, SS, TOL1,
     * TOL2,TOL3
      INTEGER I, IB2, IB, IE, IND, K1, K2, K3, LIMEXP, NEWELM, NUM
C     .. FUNCTION REFERENCES ..
      DOUBLE PRECISION X02AAF, X02ACF
C     ..
C
C           MACHINE DEPENDENT CONSTANTS
C           ------------------------
C           /LIMEXP/ IS THE MAXIMUM NUMBER OF ELEMENTS THE EPSILON
C           TABLE CAN CONTAIN. IF THIS NUMBER IS REACHED, THE UPPER
C           DIAGONAL OF THE EPSILON TABLE IS DELETED.
C
      DATA LIMEXP /50/
      EPMACH = X02AAF(1.0D0)
      OFLOW = X02ACF(1.0D0)
C
C           LIST OF MAJOR VARIABLES
C           -----------------------
C           E0     - THE 4 ELEMENTS ON WHICH THE
C           E1       COMPUTATION OF A NEW ELEMENT IN
C           E2       THE EPSILON TABLE IS BASED
C           E3                 E0
C                        E3    E1    NEW
C                              E2
C           NEWELM - NUMBER OF ELEMENTS TO BE COMPUTED IN THE NEW
C                    DIAGONAL
C           ERROR  - ERROR = ABS(E1-E0)+ABS(E2-E1)+ABS(NEW-E2)
C           RESULT - THE ELEMENT IN THE NEW DIAGONAL WITH LEAST
C                    ERROR
C
      NRES = NRES + 1
      ABSERR = OFLOW
      RESULT = EPSTAB(N)
      IF (N.LT.3) GO TO 200
      EPSTAB(N+2) = EPSTAB(N)
      NEWELM = (N-1)/2
      EPSTAB(N) = OFLOW
      NUM = N
      K1 = N
      DO 80 I=1,NEWELM
         K2 = K1 - 1
         K3 = K1 - 2
         RES = EPSTAB(K1+2)
         E0 = EPSTAB(K3)
         E1 = EPSTAB(K2)
         E2 = RES
         E1ABS = DABS(E1)
         DELTA2 = E2 - E1
         ERR2 = DABS(DELTA2)
         TOL2 = DMAX1(DABS(E2),E1ABS)*EPMACH
         DELTA3 = E1 - E0
         ERR3 = DABS(DELTA3)
         TOL3 = DMAX1(E1ABS,DABS(E0))*EPMACH
         IF (ERR2.GT.TOL2 .OR. ERR3.GT.TOL3) GO TO 20
C
C           IF E0, E1 AND E2 ARE EQUAL TO WITHIN MACHINE
C           ACCURACY, CONVERGENCE IS ASSUMED
C           RESULT = E2
C           ABSERR = ABS(E1-E0)+ABS(E2-E1)
```

```
C
         RESULT = RES
         ABSERR = ERR2 + ERR3
         GO TO 200
   20    E3 = EPSTAB(K1)
         EPSTAB(K1) = E1
         DELTA1 = E1 - E3
         ERR1 = DABS(DELTA1)
         TOL1 = DMAX1(E1ABS,DABS(E3))*EPMACH
C
C           IF TWO ELEMENTS ARE VERY CLOSE TO EACH OTHER, OMIT
C           A PART OF THE TABLE BY ADJUSTING THE VALUE OF N
C
         IF (ERR1.LT.TOL1 .OR. ERR2.LT.TOL2 .OR. ERR3.LT.TOL3) GOTO 40
         SS = 0.1D+01/DELTA1 + 0.1D+01/DELTA2 - 0.1D+01/DELTA3
         EPSINF = DABS(SS*E1)
C
C           TEST TO DETECT IRREGULAR BEHAVIOUR IN THE TABLE, AND
C           EVENTUALLY OMIT A PART OF THE TABLE ADJUSTING THE VALUE
C           OF N
C
         IF (EPSINF.GT.0.1D-03) GO TO 60
   40    N = I + I - 1
         GO TO 100
C
C           COMPUTE A NEW ELEMENT AND EVENTUALLY ADJUST
C           THE VALUE OF RESULT
C
   60    RES = E1 + 0.1D+01/SS
         EPSTAB(K1) = RES
         K1 = K1 - 2
         ERROR = ERR2 + DABS(RES-E2) + ERR3
         IF (ERROR.GT.ABSERR) GO TO 80
         ABSERR = ERROR
         RESULT = RES
   80 CONTINUE
C
C           SHIFT THE TABLE
C
  100 IF (N.EQ.LIMEXP) N = 2*(LIMEXP/2) - 1
      IB = 1
      IF ((NUM/2)*2.EQ.NUM) IB = 2
      IE = NEWELM + 1
      DO 120 I=1,IE
         IB2 = IB + 2
         EPSTAB(IB) = EPSTAB(IB2)
         IB = IB2
  120 CONTINUE
      IF (NUM.EQ.N) GO TO 160
      IND = NUM - N + 1
      DO 140 I=1,N
         EPSTAB(I) = EPSTAB(IND)
         IND = IND + 1
  140 CONTINUE
  160 IF (NRES.GE.4) GO TO 180
      RES3LA(NRES) = RESULT
      ABSERR = OFLOW
      GO TO 200
C
C           COMPUTE ERROR ESTIMATE
C
  180 ABSERR = DABS(RESULT-RES3LA(3)) + DABS(RESULT-RES3LA(2)) +
     *DABS(RESULT-RES3LA(1))
      RES3LA(1) = RES3LA(2)
      RES3LA(2) = RES3LA(3)
      RES3LA(3) = RESULT
  200 ABSERR = DMAX1(ABSERR,5.0D+00*EPMACH*DABS(RESULT))
      RETURN
      END
C
C
      SUBROUTINE D01AJZ(F, A, B, RESULT, ABSERR, RESABS, RESASC)
C                    SUBROUTINE D01AJZ, PART OF PEM (VERSION 82360).
C
C     MARK 8 RELEASE. NAG COPYRIGHT 1979
C     BASED ON QUADPACK ROUTINE QUARUL
C     ******************************************************
```

```
C
C            PURPOSE
C               TO COMPUTE I = INTEGRAL OF F OVER (A,B), WITH ERROR
C                              ESTIMATE
C                          J = INTEGRAL OF ABS(F) OVER (A,B)
C
C            CALLING SEQUENCE
C               CALL D01AJZ (F,A,B,RESULT,ABSERR,RESABS,RESASC)
C
C            PARAMETERS
C               F      - FUNCTION SUBPROGRAM DEFINING THE INTEGRAND
C                        FUNCTION F(X). THE ACTUAL NAME FOR F NEEDS
C                        TO BE DECLARED E X T E R N A L IN THE
C                        CALLING PROGRAM
C
C               A      - LOWER LIMIT OF INTEGRATION
C
C               B      - UPPER LIMIT OF INTEGRATION
C
C               RESULT - APPROXIMATION TO THE INTEGRAL I.
C                        RESULT IS CALCULATED BY APPLYING
C                        THE 21-POINT GAUSS-KRONROD RULE
C                        (RESK), OBTAINED BY OPTIMAL
C                        ADDITION OF ABSCISSAE TO THE
C                        10-POINT GAUSS  RULE (RESG).
C
C               ABSERR - ESTIMATE OF THE MODULUS OF THE
C                        ABSOLUTE ERROR, WHICH SHOULD NOT
C                        EXCEED ABS(I-RESULT)
C               RESABS - APPROXIMATION TO THE INTEGRAL J
C
C               RESASC - APPROXIMATION TO THE INTEGRAL OF
C                        ABS(F-I/(B-A)) OVER (A,B)
C
C     ********************************************************
C     .. SCALAR ARGUMENTS ..
      DOUBLE PRECISION A, ABSERR, B, RESABS, RESASC, RESULT
C     .. FUNCTION ARGUMENTS ..
      DOUBLE PRECISION F
C     ..
C     .. LOCAL SCALARS ..
      DOUBLE PRECISION ABSC, CENTRE, DHLGTH, EPMACH, FC, FSUM, FVAL1,
     * FVAL2,HLGTH, RESG, RESK, RESKH, UFLOW
      INTEGER J
C     .. LOCAL ARRAYS ..
      DOUBLE PRECISION FV1(10), FV2(10), WG(10), WGK(11), XGK(11)
C     .. FUNCTION REFERENCES ..
      DOUBLE PRECISION X02AAF, X02ABF
C     ..
C
C            THE ABSCISSAE AND WEIGHTS ARE GIVEN FOR THE
C            INTERVAL (-1,1) . BECAUSE OF SYMMETRY ONLY THE
C            POSITIVE ABSCISSAE AND THEIR CORRESPONDING
C            WEIGHTS ARE GIVEN.
C            XGK    - ABSCISSAE OF THE 21-POINT GAUSS-KRONROD RULE
C                     XGK(2), XGK(4), .... ABSCISSAE OF THE 10-POINT
C                     GAUSS RULE
C                     XGK(1), XGK(3), .... ABSCISSAE WHICH
C                     ARE OPTIMALLY ADDED TO THE 10-POINT
C                     GAUSS RULE
C            WGK    - WEIGHTS OF THE 21-POINT GAUSS-KRONROD RULE
C            WG     - WEIGHTS OF THE 10-POINT GAUSS RULE,
C                     CORRESPONDING TO THE ABSCISSAE XGK(2),
C                     XGK(4), ... WG(1), WG(3), ... ARE SET
C                     TO ZERO.
C
      DATA XGK(1), XGK(2), XGK(3), XGK(4), XGK(5), XGK(6), XGK(7),XGK(8)
     *, XGK(9), XGK(10), XGK(11) /0.99565716302580808073552728070D+00,
     *0.97390652851717172007796401210D+00,
     *0.93015749135570822600120718010D+00,
     *0.86506336668898451073209668840D+00,
     *0.78081772658641689706371757830D+00,
     *0.67940956829902440623432736510D+00,
     *0.56275713466860468333900009930D+00,
     *0.43339539412924719079926594320D+00,
     *0.29439286270146019813112660310D+00,
     *0.14887433898163121088482600110D+00,0.0D0/
```

```
      DATA WGK(1), WGK(2), WGK(3), WGK(4), WGK(5), WGK(6), WGK(7),WGK(8)00042310
     *, WGK(9), WGK(10), WGK(11) /0.1169463886737187427806439606D-01,   00042320
     *0.3255816230796472747881897246D-01,                               00042330
     *0.5475589657435199603138130024D-01,                               00042340
     *0.7503967481091995276704314092D-01,                               00042350
     *0.9312545458369760553506546508D-01,                               00042360
     *0.1093871588022976418992105903D+00,                               00042370
     *0.1234919762620658510779581098D+00,                               00042380
     *0.1347092173114733259280540018D+00,                               00042390
     *0.1427759385770600807970942731D+00,                               00042400
     *0.1477391049013384913748415160D+00,                               00042410
     *0.1494455540029169056649364684D+00/                               00042420
      DATA WG(1), WG(2), WG(3), WG(4), WG(5), WG(6), WG(7), WG(8),WG(9),00042430
     * WG(10) /0.0D0,0.6667134430868813759356880989D-01,0.0D0,          00042440
     *0.1494513491505805931457763397D+00,0.0D0,                         00042450
     *0.2190863625159820439955349342D+00,0.0D0,                         00042460
     *0.2692667193099963550912269216D+00,0.0D0,                         00042470
     *0.2955242247147528701738929947D+00/                               00042480
      EPMACH = X02AAF(1.0D0)                                            00042490
      UFLOW = X02ABF(1.0D0)                                             00042500
C                                                                       00042510
C           LIST OF MAJOR VARIABLES                                     00042520
C           ----------------------                                      00042530
C           CENTRE - MID POINT OF THE INTERVAL                          00042540
C           HLGTH  - HALF LENGTH OF THE INTERVAL                        00042550
C           ABSC   - ABSCISSA                                           00042560
C           FVAL*  - FUNCTION VALUE                                     00042570
C           RESG   - 10-POINT GAUSS FORMULA                             00042580
C           RESK   - 21-POINT GAUSS-KRONROD FORMULA                     00042590
C           RESKH  - APPROXIMATION TO MEAN VALUE OF F OVER              00042600
C                    (A,B), I.E. TO I/(B-A)                             00042610
C                                                                       00042620
      CENTRE = 0.5D+00*(A+B)                                            00042630
      HLGTH = 0.5D+00*(B-A)                                             00042640
      DHLGTH = DABS(HLGTH)                                              00042650
C                                                                       00042660
C           COMPUTE THE 21-POINT GAUSS-KRONROD APPROXIMATION TO         00042670
C           THE INTEGRAL, AND ESTIMATE THE ABSOLUTE ERROR               00042680
C                                                                       00042690
      RESG = 0.0D+00                                                    00042700
      FC = F(CENTRE)                                                    00042710
      RESK = WGK(11)*FC                                                 00042720
      RESABS = DABS(RESK)                                               00042730
      DO 20 J=1,10                                                      00042740
         ABSC = HLGTH*XGK(J)                                            00042750
         FVAL1 = F(CENTRE-ABSC)                                         00042760
         FVAL2 = F(CENTRE+ABSC)                                         00042770
         FV1(J) = FVAL1                                                 00042780
         FV2(J) = FVAL2                                                 00042790
         FSUM = FVAL1 + FVAL2                                           00042800
         RESG = RESG + WG(J)*FSUM                                       00042810
         RESK = RESK + WGK(J)*FSUM                                      00042820
         RESABS = RESABS + WGK(J)*(DABS(FVAL1)+DABS(FVAL2))             00042830
   20 CONTINUE                                                          00042840
      RESKH = RESK*0.5D+00                                              00042850
      RESASC = WGK(11)*DABS(FC-RESKH)                                   00042860
      DO 40 J=1,10                                                      00042870
         RESASC = RESASC + WGK(J)*(DABS(FV1(J)-RESKH)+DABS(FV2(J)-RESKH)00042880
     *   )                                                              00042890
   40 CONTINUE                                                          00042900
      RESULT = RESK*HLGTH                                               00042910
      RESABS = RESABS*DHLGTH                                            00042920
      RESASC = RESASC*DHLGTH                                            00042930
      ABSERR = DABS((RESK-RESG)*HLGTH)                                  00042940
      IF (RESASC.NE.0.0D+00) ABSERR = RESASC*DMIN1(0.1D+01,(0.2D+03*    00042950
     *ABSERR/RESASC)**1.5D0)                                            00042960
      IF (RESABS.GT.UFLOW/(0.5D+02*EPMACH)) ABSERR =DMAX1(EPMACH*RESABS*00042970
     *0.5D+02,ABSERR)                                                   00042980
      RETURN                                                            00042990
      END                                                               00043000
C                                                                       00043010
C                                                                       00043020
      INTEGER FUNCTION P01AAF(IFAIL, ERROR, SRNAME)                     00043030
C                         FUNCTION P01AAF, PART OF PEM (VERSION 82360). 00043040
C                                                                       00043050
C     MARK 1 RELEASE.  NAG COPYRIGHT 1971                               00043060
C     MARK 3 REVISED                                                    00043070
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C     MARK 4A REVISED, IER-45                                           00043080
C     MARK 4.5 REVISED                                                  00043090
C     MARK 7 REVISED (DEC 1978)                                         00043100
C     RETURNS THE VALUE OF ERROR OR TERMINATES THE PROGRAM.             00043110
      INTEGER ERROR, IFAIL, NOUT                                        00043120
C$P 1                                                                   00043130
      DOUBLE PRECISION SRNAME                                           00043140
C     TEST IF NO ERROR DETECTED                                         00043150
      IF (ERROR.EQ.0) GO TO 20                                          00043160
C     DETERMINE OUTPUT UNIT FOR MESSAGE                                 00043170
      CALL X04AAF (0,NOUT)                                              00043180
C     TEST FOR SOFT FAILURE                                             00043190
      IF (MOD(IFAIL,10).EQ.1) GO TO 10                                  00043200
C     HARD FAILURE                                                      00043210
      WRITE (NOUT,99999) SRNAME, ERROR                                  00043220
C     STOPPING MECHANISM MAY ALSO DIFFER                                00043230
      STOP                                                              00043240
C     SOFT FAIL                                                         00043250
C     TEST IF ERROR MESSAGES SUPPRESSED                                 00043260
   10 IF (MOD(IFAIL/10,10).EQ.0) GO TO 20                               00043270
      WRITE (NOUT,99999) SRNAME, ERROR                                  00043280
   20 P01AAF = ERROR                                                    00043290
      RETURN                                                            00043300
99999 FORMAT (1H0, 38HERROR DETECTED BY NAG LIBRARY ROUTINE , A8,       00043310
     * 11H - IFAIL = , I5//)                                            00043320
      END                                                               00043330
C                                                                       00043340
C                                                                       00043350
      DOUBLE PRECISION FUNCTION X02AAF(X)                               00043360
C                        FUNCTION X02AAF, PART OF PEM (VERSION 82360).  00043370
C                                                                       00043380
C     NAG COPYRIGHT 1975                                                00043390
C     MARK 4.5 RELEASE                                                  00043400
      DOUBLE PRECISION X                                                00043410
C     * EPS *                                                           00043420
C                                                                       00043430
C     IBM DOUBLE PRECISION VERSION                                      00043440
C                                                                       00043450
C     RETURNS THE VALUE EPS WHERE EPS IS THE SMALLEST                   00043460
C     POSITIVE                                                          00043470
C     NUMBER SUCH THAT 1.0 + EPS > 1.0                                  00043480
C     THE X PARAMETER IS NOT USED                                       00043490
C     FOR ICL 1900                                                      00043500
C     X02AAF = 2.0**(-37.0)                                             00043510
C     FOR IBM 360/370                                                   00043520
C     X02AAF = 2.0D0**(-52.0D0)                                         00043530
      DOUBLE PRECISION Z                                                00043540
      DIMENSION ZZ(2)
      EQUIVALENCE (ZZ(1),Z)
      DATA ZZ /O171410000000,0000000000000/
C     DATA Z/Z3410000000000000/                                         00043550
      X02AAF = Z                                                        00043560
      RETURN                                                            00043570
      END                                                               00043580
C                                                                       00043590
C                                                                       00043600
      DOUBLE PRECISION FUNCTION X02ABF(X)                               00043610
C                        FUNCTION X02ABF, PART OF PEM (VERSION 82360).  00043620
C                                                                       00043630
C     NAG COPYRIGHT 1975                                                00043640
C     MARK 4.5 RELEASE                                                  00043650
      DOUBLE PRECISION X                                                00043660
C     * RMIN *                                                          00043670
C                                                                       00043680
C     IBM DOUBLE PRECISION VERSION                                      00043690
C                                                                       00043700
C     RETURNS THE VALUE OF THE SMALLEST POSITIVE REAL FLOATING-         00043710
C     POINT NUMBER EXACTLY REPRESENTABLE ON THE COMPUTER                00043720
C     THE X PARAMETER IS NOT USED                                       00043730
C     FOR ICL 1900                                                      00043740
C     X02ABF = 2.0**(-257.0)                                            00043750
C     FOR IBM 360/370                                                   00043760
C     X02ABF = 16.0D0**(-65.0D0)                                        00043770
      DOUBLE PRECISION Z                                                00043780
      DIMENSION ZZ(2)
      EQUIVALENCE (ZZ(1),Z)
      DATA ZZ /0000110000000,0000000000000/
```

```
C     DATA Z/Z0010000000000000/                                         00043790
      X02ABF = Z                                                        00043800
      RETURN                                                            00043810
      END                                                               00043820
C                                                                       00043830
C                                                                       00043840
      DOUBLE PRECISION FUNCTION X02ACF(X)                               00043850
C                          FUNCTION X02ACF, PART OF PEM (VERSION 82360). 00043860
C                                                                       00043870
C     NAG COPYRIGHT 1975                                                00043880
C     MARK 4.5 RELEASE                                                  00043890
      DOUBLE PRECISION X                                                00043900
C     * RMAX *                                                          00043910
C                                                                       00043920
C     IBM DOUBLE PRECISION VERSION                                      00043930
C                                                                       00043940
C     RETURNS THE VALUE OF THE LARGEST POSITIVE REAL  FLOATING-         00043950
C     POINT NUMBER REPRESENTABLE ON THE COMPUTER                        00043960
C     FOR ICL 1900                                                      00043970
C     X02ACF = (2.0 - 2.0**(-36.0))*2.0**254.0                          00043980
C     FOR IBM 360/370                                                   00043990
C     X02ACF = (1.0D0-16.0D0**(-14.0D0))*16.0D0**63.0D0                 00044000
      DOUBLE PRECISION Z                                                00044010
      DIMENSION ZZ(2)
      EQUIVALENCE (ZZ(1),Z)
      DATA ZZ /0377777777777,0777777777777/
C     DATA Z/Z7FFFFFFFFFFFFFFF/                                         00044020
      X02ACF = Z                                                        00044030
      RETURN                                                            00044040
      END                                                               00044050
C                                                                       00044060
C                                                                       00044070
      SUBROUTINE X04AAF(I,NERR)                                         00044080
C                    SUBROUTINE X04AAF, PART OF PEM (VERSION 82360).    00044090
C                                                                       00044100
C     MARK 7 RELEASE. NAG COPYRIGHT 1978                                00044110
C     MARK 7C REVISED IER-190 (MAY 1979)                                00044120
C     IF I = 0, SETS NERR TO CURRENT ERROR MESSAGE UNIT NUMBER          00044130
C     (STORED IN NERR1).                                                00044140
C     IF I = 1, CHANGES CURRENT ERROR MESSAGE UNIT NUMBER TO            00044150
C     VALUE SPECIFIED BY NERR.                                          00044160
C                                                                       00044170
C     *** NOTE ***                                                      00044180
C     THIS ROUTINE ASSUMES THAT THE VALUE OF NERR1 IS SAVED             00044190
C     BETWEEN CALLS.  IN SOME IMPLEMENTATIONS IT MAY BE                 00044200
C     NECESSARY TO STORE NERR1 IN A LABELLED COMMON                     00044210
C     BLOCK /AX04AA/ TO ACHIEVE THIS.                                   00044220
C                                                                       00044230
C     .. SCALAR ARGUMENTS ..                                            00044240
      INTEGER I, NERR                                                   00044250
C     ..                                                                00044260
C     .. LOCAL SCALARS ..                                               00044270
      INTEGER NERR1                                                     00044280
C     ..                                                                00044290
      DATA NERR1 /6/                                                    00044300
      IF (I.EQ.0) NERR = NERR1                                          00044310
      IF (I.EQ.1) NERR1 = NERR                                          00044320
      RETURN                                                            00044330
      END                                                               00044340
**

@BRKPT  PRINT$
```